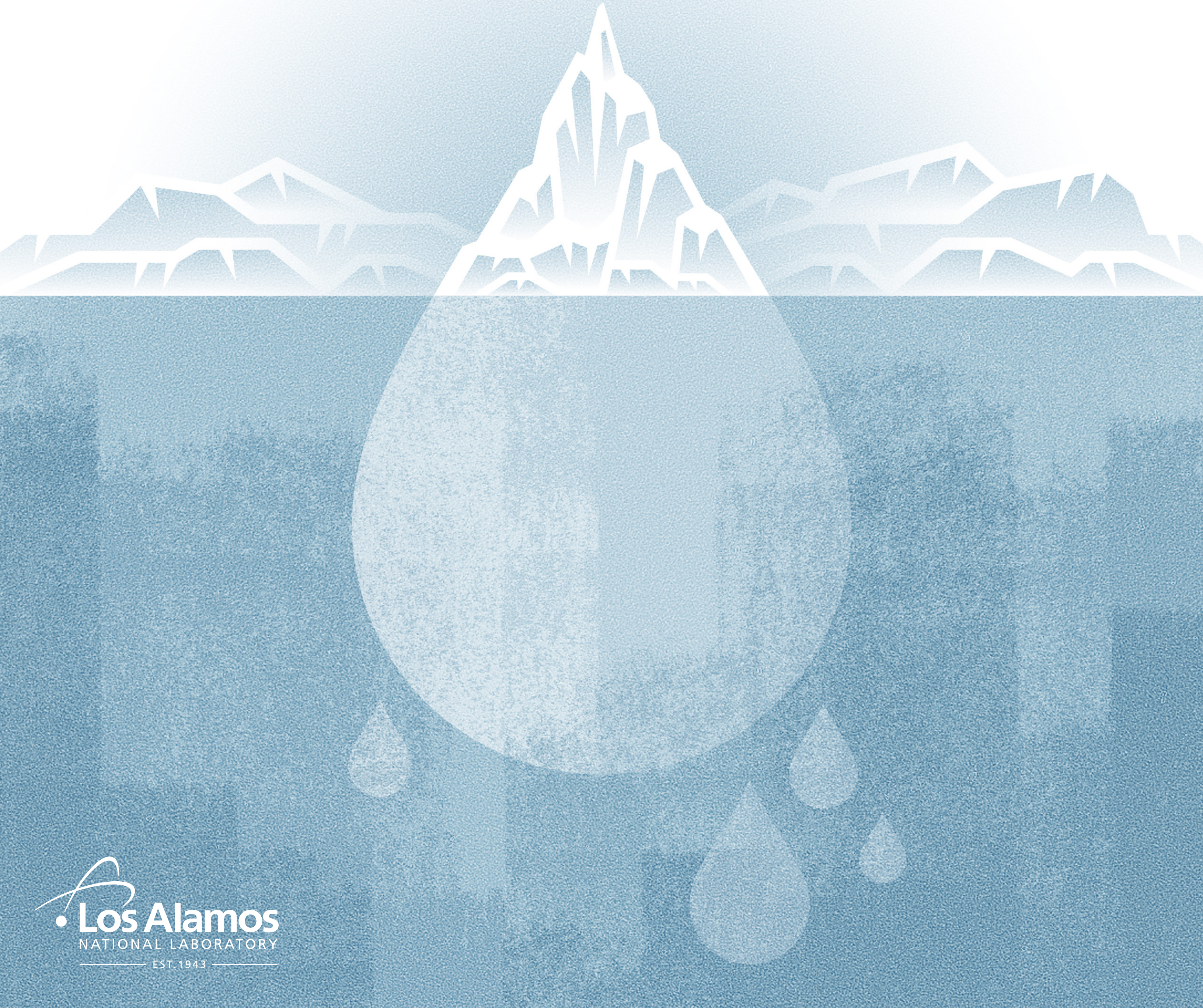
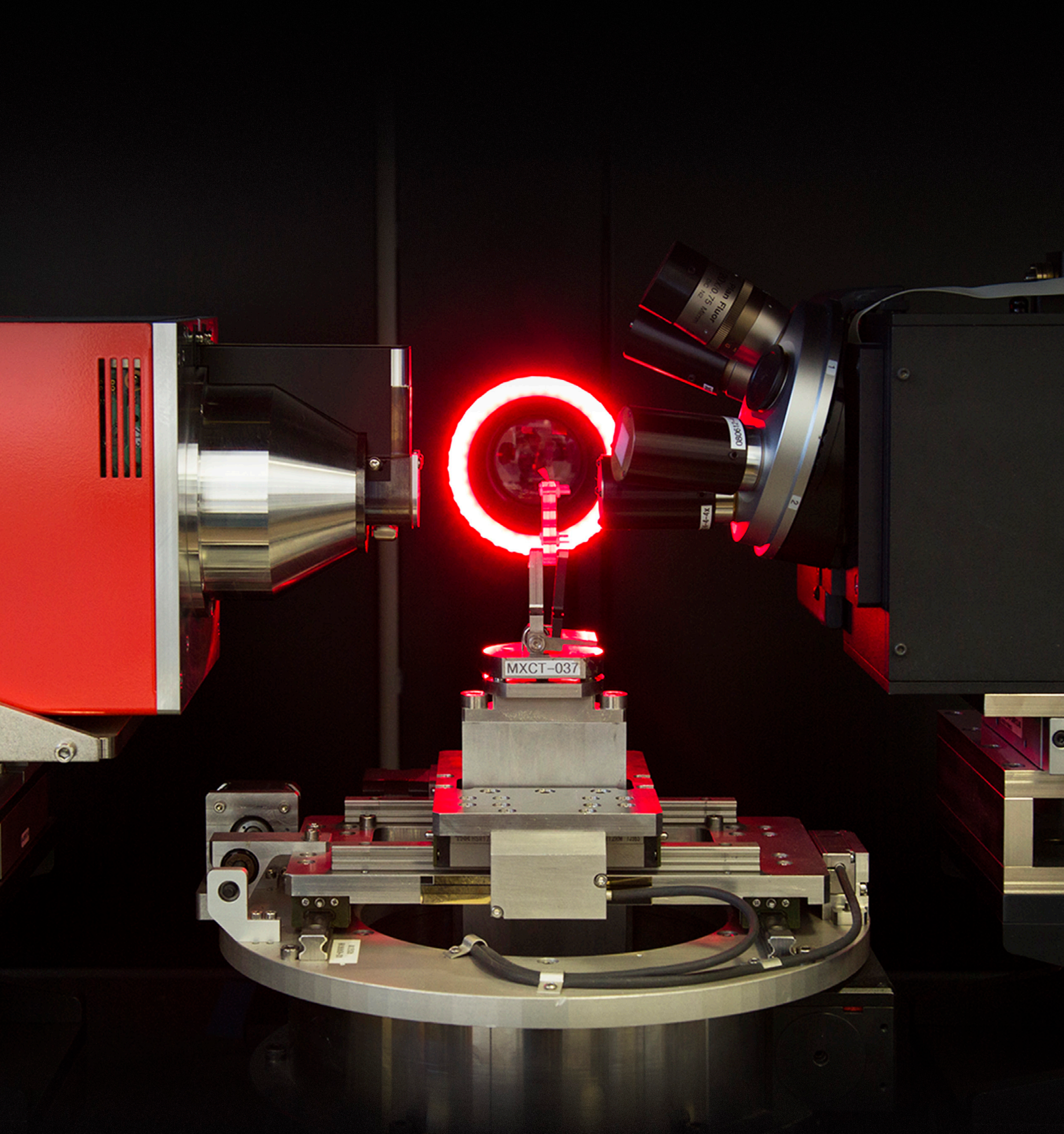
Los Alamos Science and Technology Magazine | December 2016

1663

Sustainable transportation
Cancer's fingerprints
Big science with little lasers
Deflecting deadly comets

AN ICE SHEET'S DEMISE





The quest to build the best fuel cell for automobiles involves developing and understanding new materials. Here, a prototype membrane-electrode assembly is being evaluated by micro x-ray computed tomography. The technique uses x-rays to create multiple cross-section images that can be digitally combined to recreate a virtual model of a physical object. The result is a highly detailed 3D image of the whole assembly and its microstructure, produced without damaging any part of the precious prototype. (The glowing red ring is the source of illumination for the side-view camera to help adjust and align the sample.) See "Driving Sustainability" on page 16.

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LOS ALAMOS SCIENCE AND TECHNOLOGY MAGAZINE

About the Cover:

Most of Greenland, which is more than three times the size of Texas, is covered by an ice sheet rising more at its highest point than 10,000 feet above the underlying bedrock. The ice sheet covering Antarctica contains about 10 times more ice still, with the two ice sheets combined holding about two thirds of all the fresh water on Earth. Greenland's ice sheet is currently melting about twice as fast as Antarctica's, and if it were to go (over a thousand or more years), the meltwater would raise global sea levels by more than 20 feet—enough to submerge at least part of most coastal cities (as they exist today) and enormous swaths of low-lying lands all over the world. Recent Los Alamos research indicates that, based on humanity's current carbon-emissions trajectory, the fate of the Greenland ice sheet for millennia to come will be locked in sometime this century, possibly within just a few decades.

About Our Name:

During World War II, all that the outside world knew of Los Alamos and its top-secret laboratory was the mailing address—P. O. Box 1663, Santa Fe, New Mexico. That box number, still part of our address, symbolizes our historic role in the nation's service.

About the LDRD Logo:

Laboratory Directed Research and Development (LDRD) is a competitive internal program by which Los Alamos National Laboratory is authorized by Congress to invest in research and development that is both highly innovative and vital to national interests. Whenever *1663* reports on research that received support from LDRD, this logo appears at the end of the article.

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SPOTLIGHTS

Diverting Doomsday

IN JULY OF 1994, COMET SHOEMAKER-LEVY 9 CRASHED into Jupiter. Astronomers watched in awe as dozens of comet fragments bombarded the giant planet's southern hemisphere and debris clouds billowed to 12,000 kilometers (km) across, roughly the same diameter as the earth. It was the first time anyone had witnessed two major celestial bodies collide within our solar system, leading stargazers around the world to the same apprehension: what if it had been Earth?

The drama on Jupiter was a wake-up call, underscoring the reality that demise-by-comet isn't just for dinosaurs. Humanity has had 22 years since then to put into place a planetary defense system capable of deterring a doomsday comet. And yet, today, no such system exists.

Roughly every million years, an object measuring at least 1 km across hits the earth. And roughly every 100 million years, an object measuring at least 10 km across hits it; one of these is thought to have caused the extermination of the dinosaurs 66 million years ago. Comets on orbits of more than 200 years are called long-period comets and are believed to come from the Oort cloud, a spherical region full of icy objects surrounding our solar system. These objects occasionally get dislodged from their orbit within the Oort cloud and begin to fall toward the inner solar system. We earthlings call them comets when they get close enough to the sun to begin to vaporize; the boiled-off surface material is pushed outward by the solar wind, creating their characteristic tails.

Comets, especially long-period comets, are more worrisome than asteroids in terms of planetary defense for several reasons. First, they are the fastest objects in our solar system, which doesn't leave much time for defensive measures—18 months at most from the time of a comet's discovery. Second, their orbits are so long they usually come around only once on the timescale of our civilization, making them impossible to anticipate based on a prior appearance. Third, they tend to be quite large, ranging 1–40 km in diameter. If a long-period comet just 10 km across were to hit Earth, it would deliver over a billion times the combined energy of the nuclear bombs that devastated Hiroshima and Nagasaki.

"It's a great cosmic billiards game out there," says Los Alamos plasma physicist Glen Wurden, "and there *is* a comet somewhere that *is* going to hit us. We just don't know when—it could be in millions of years or it could be tomorrow." In his plasma research lab, Wurden, who is also an avid backyard astronomer, chucks tiny pieces of ice into plasmas, making what amount to very, very small comets. This got him thinking about very, very big comets, and he came up with a wild idea.

There isn't much to be done, defense-wise, about a comet's size or orbit, but Wurden's idea is to change its trajectory. It would require a rocket with enough speed to close the distance between Earth and the comet quickly, typically in about half the time until impact. No such rocket exists, but Wurden believes it could, if scientists put their minds and skills to the task.

It would have to be nuclear. Only a rocket propelled by thermonuclear fusion would have the necessary combination of power and speed to get there in time, and only a thermonuclear warhead would deliver the bump needed to change the colossal comet's trajectory. This is both convenient and inconvenient at once. It's convenient because some of the technology already exists, and scientists, especially Los Alamos scientists, have the nuclear skills and technical know-how to pursue such a rocket. It's inconvenient, however, because there are two international treaties that would require amending: one to allow nuclear devices in temporary orbit around Earth and another to allow detonation of nuclear explosives in space. Both of these are presently prohibited.

Comet Lovejoy (C/2013 R1) over Los Alamos, New Mexico, December 2, 2013.
CREDIT: Glen Wurden

Should the legalities get resolved, the comet interceptor would accelerate continuously as the distance to the comet narrows then detonate the explosive when the rocket is about 1 km away. The explosion wouldn't destroy the comet, but the radiation from the explosion would burn and boil material off the side of the comet, changing its mass and momentum. In a scenario where the comet is intercepted six months before its predicted calamity, Wurden calculated that the explosion would need to exact a change of 10 meters per second to amount to a 150,000-km difference by the time the comet whizzes past Earth. That's still a close shave, but humanity would behold a spectacle in the night sky rather than the end of days.

Wurden points out that although fusion rocket engines don't technically exist yet, preliminary designs do exist, and Los Alamos National Laboratory, with its nuclear, space travel, engineering, and computational expertise, is ideally equipped for the tremendous task of answering this cometary call to arms.

But then there's the price tag to consider. What is the insurance premium for a planet and all of its inhabitants? Wurden estimates an annual budget of $10 billion in perpetuity. That may seem high, but a single aircraft carrier runs in the neighborhood of $13 billion. Besides, we would split the check with other space-faring nations, so our cost would be just a fraction of the total.

"It's not chicken little," Wurden emphasizes. "A hit in the Pacific Ocean would create a tsunami that would cream every city on the Pacific Rim. Dust and debris would make short work of the rest of humanity. There are some catastrophes, like volcano eruptions, that we really can't do anything about. This isn't one of them."

It's a wild idea indeed, but perhaps it shouldn't be.

— Eleanor Hutterer

Renegade Particles

NEUTRINOS LOVE CONTROVERSY. AND EARLIER THIS YEAR, evidence for a new type of neutrino, whose existence was first implied by a Los Alamos experiment in the 1990s, was both amplified *and* refuted.

Neutrinos, lightweight and thoroughly invisible subatomic particles, weren't even supposed to exist until it was discovered that the radioactive beta-decay process needs them to conserve energy and momentum. Then they weren't supposed to have any mass, until it was discovered that they spontaneously transform, or "oscillate," from one variety, or "flavor," to another, which requires mass. They certainly weren't supposed to come in more than three flavors (no other fundamental matter particle seems to) or behave asymmetrically with respect to their antimatter counterparts, but now both acts of defiance may be necessary to explain a resilient collection of measurement anomalies.

All along, Los Alamos has been at the forefront of the neutrino oscillation mystery. It began with the Lab's Liquid Scintillator Neutrino Detector (LSND) experiment—for a long time, the only outlier in a suite of otherwise consistent neutrino-oscillation experiments. LSND's results agreed with those of other experiments, indicating that neutrinos oscillate from one flavor to another. But the oscillation parameters depend on the relative neutrino masses, and LSND's measurements implied much larger masses than those obtained elsewhere. Like so many things from the 90s (sagging pants and transparent cola spring to mind), the LSND results didn't make much sense.

So vexing were the results that a follow-up experiment was commissioned expressly to confirm or disprove them. That experiment, MiniBooNE (Mini Booster Neutrino Experiment)—designed in part by Los Alamos scientists and operating at the Fermi National Accelerator Laboratory (Fermilab) in Illinois since 2002—proved everybody right. In neutrino mode, MiniBooNE initially agreed with the consensus of neutrino experiments, producing results consistent with small neutrino masses. But when it used antineutrinos instead, it agreed with LSND, also an antineutrino experiment, requiring much larger neutrino masses. Because particle and antiparticle masses are identical, MiniBooNE and LSND together require additional neutrino flavors with masses greatly exceeding those of the three original flavors. Yet other high-precision cosmological data sets strongly restrict the number of active neutrino flavors to just the original three.

To fit the bill, then, physicists suggested there might be one or more additional flavors of *sterile* neutrino, in addition to the three active flavors. Sterile neutrinos are so named because they would never interact with anything (except via gravity, to which nothing is immune). That means they wouldn't show up in the cosmological data but could still appear when neutrinos oscillate from one flavor to another. Then, when a known number of neutrinos is fired at a detector, and the detector registers fewer than it's supposed to, researchers might infer that the missing neutrinos oscillated from an active flavor to a sterile one, as though the particles had oscillated right out of existence.

Such disappearances have been reported periodically at experiments around the world, especially those using antineutrinos produced by nuclear power reactors. Earlier this year, the Daya Bay reactor-based experiment in China reported the highest-precision measurement to date of the possible sterile-neutrino signal. Yet by late summer, a large neutrino observatory called IceCube (so named because it is set within a cubic kilometer of ice at the South Pole), announced that it had firmly ruled out the sterile neutrino within the expected mass range—that is, for the quantity directly probed, denoted Δm^2, between 0.1 and 1.0 square electronvolts (eV^2). A sterile neutrino with a mass outside that range could still exist according to the IceCube data, and possibly explain the LSND signal, but it wouldn't easily explain the MiniBooNE data. (A sterile neutrino measurement of $\Delta m^2 = 1.75\ eV^2$ might satisfy all the data, barely; that will be investigated by new experiments over the next year.)

So what is a major research institution with a conflicted history in neutrino physics to do in the face of such consistently inconsistent results? Double down to root out the source of the discrepancy, that's what. Los Alamos is currently working on three more detectors—ICARUS (Imaging Cosmic And Rare Underground Signals), SBND (Short-Baseline Near Detector), and MicroBooNE—to be staged at varying distances along the same neutrino beamline at Fermilab with MiniBooNE.

Each of the three is a liquid-argon time-projection chamber, a new and advanced technology for capturing complex particle collisions and reconstructing all the particle trajectories. This will provide more comprehensive information on neutrino events than physicists have had in the past. In addition, Los Alamos recently finished constructing its MiniCAPTAIN detector (Mini Cryogenic Apparatus for Precision Tests of Argon Interactions with Neutrinos) and installed it in an accelerator beam at the Los Alamos Neutron Science Center. Also a liquid-argon detector, it will be used to reconstruct neutron interactions for the purpose of improving scientists' understanding of the detector response, thereby enabling a more accurate interpretation of upcoming neutrino events in the new detectors at Fermilab.

"I think we're closing in on the biggest mystery in particle physics—the one undeniable dent in the field's otherwise phenomenally successful Standard Model," says Richard Van de Water, one of the Los Alamos architects of MiniBooNE. "But the good news, amid all the seemingly conflicting data, is that *something* is definitely going on. There is new physics at work here, and nature is teasing us with a glimpse of it."

That new physics may help answer some enduring scientific mysteries. One such mystery is the very existence of matter: some fundamental asymmetry in the laws of physics—perhaps like the apparent discrepancy between neutrino and antineutrino oscillation experiments—is needed to explain why our universe contains plenty of matter but not antimatter. Without such an asymmetry, matter and antimatter should have come to exist in equal numbers in the early universe and then annihilated each other, effectively leaving none of either. It's an unresolved glitch in the Standard Model of particle physics that may be responsible for the existence of, well, everything.

In addition, the new physics might help identify the universe's dark matter. If a heavy enough sterile neutrino exists, it would do exactly what dark matter does: gather into large, invisible clumps in space that exert a strong gravitational influence on stars and galaxies. And even if the dark matter particle is something other than a sterile neutrino, as most theories would suggest, the new liquid-argon detectors at Fermilab may be able to see evidence for it. In fact, Los Alamos is working on a secondary mission for the new detectors, repurposing them to search for dark matter in a lower mass range than most dark matter experiments probe.

So with the sterile neutrino, matter-antimatter asymmetry, and dark matter mysteries on the line, scientists are ratcheting up the investigation. Time will tell how much longer neutrinos can keep their controversy alive. LDRD

—Craig Tyler

Particle track from a neutrino event candidate inside the MicroBooNE liquid-argon detector: The red dot is the point where an incoming neutrino interacted with an argon nucleus, generating a spray of other particles. Entering from the left, the neutrino is uncharged and therefore unseen; outgoing straight lines are charged particles, and the sequence of squiggly lines angling downward represents photons that convert into electron-antielectron pairs, which, by virtue of their small masses, are quickly buffeted about by multiple scatterings with the surrounding atoms. Streaks perpendicular to the particle spray represent unrelated background activity. By studying the outgoing particle tracks, researchers can reconstruct the energy and flavor of the incident neutrino.

CREDIT: MicroBooNE collaboration

CREDIT: Dave Barfield

IN THEIR OWN WORDS

Laboratory physicist **ALBERT MIGLIORI** describes a career solving scientific mysteries for national security.

SEPTEMBER 1973.

It's late afternoon, the sky is black, and Jemez mountain lightning and thunder accompany a monsoon rain as I wind my way up the main hill road to Los Alamos for the first time, stunned by the view that confirms my decision to accept a Los Alamos Director's Postdoctoral Fellow position. Of course, I am also terrified to be starting at a serious research institution. A few months earlier, I had completed my Ph.D. in condensed matter physics, and, as fate would have it, the Vietnam war had ended, releasing me from a two-year obligation to serve as a 1st Lieutenant in the U.S. Army Signal Corps on combat duty. I'd also just turned down a permanent position with another national laboratory, hoping to land the job at Los Alamos.

Graduate school had given me a superb education in hard-core, hands-dirty experimental physics, and I was hooked, then and now. During that first decade at Los Alamos, I had a blast. I was promoted to permanent staff and began working with John Wheatley, a famous low-temperature physicist, on acoustic engines—an idea I had from the operation of tuned exhausts in two-stroke motorcycle engines. Wheatley ran with this, and I was barely able to hang on, but this was how I got my start with acoustic methods.

After Wheatley's death, I headed back to condensed-matter physics. Around that same time, the physics world was turned upside down by the discovery of high-temperature superconductors. Unlike all previously discovered superconductors in which electrical current flows resistance-free below a critical temperature T_c close to absolute zero, high-T_c superconductors function at more accessible temperatures, perhaps someday without any cooling at all. (This would be nothing short of a technological revolution, and the quest for it continues to this day.)

With my doctoral work on superconductivity and the thermodynamics I had picked up since, I knew that a crucial high-T_c measurement would be of the superconductor's bulk-modulus discontinuity at the superconducting transition—a required sharp change in the material's elastic properties at T_c. So I began to develop a technique for carrying out that measurement, resonant ultrasound spectroscopy (RUS), not knowing at the time that geologists had been doing the same. Lucky for me (not so much for them), my background in electronics and Los Alamos's advanced computing capabilities were such that my colleagues and I were able to develop this tool, hardware and software, to the point where it is now widely used. (In crediting the pioneering work by geologists that I only later found out about, I was quoted in *Physics Today* as saying, "Six months in the lab can save you a day in the library.")

Although a decade passed before we could get good enough high-T_c material to make the measurement, RUS became a useful ultrasound technique, and I was asked if I'd like to use it to measure plutonium. Talk about low-hanging fruit! The state of elastic stiffness measurements on plutonium was both a total mess and critically important to the Laboratory's national security mission. And who could compete with us? So off I went to Tech Area 55 to see if plutonium rang like the bell we needed, which is what RUS actually measures—the ring frequencies of a solid object.

To our amazement, plutonium was an ideal RUS target; the first scan gave us all goosebumps, it was so good. During the next several years, we knocked off the elastic moduli over

I AM ADDICTED TO THE VISCERAL REACTION OF DISCOVERING SOMETHING THAT, UNTIL THAT MOMENT, NO ONE ON THE ENTIRE PLANET KNEW.

the full range of existence of several of plutonium's crystal configurations: alpha, gamma, then beta. At the same time, we studied gallium-stabilized delta plutonium and, for all the measurements, got the error bars down to the size of the data points themselves. (Delta-phase plutonium, naturally occurring only well above room temperature, is useful because it is ductile, rather than brittle like the room-temperature alpha phase. A little added gallium brings the delta phase down to room temperature.)

Every few years along the way, I redesigned the electronics, getting better and better performance, until we realized that we had reached a noise-limited measurement precision of about one part in 10^8. We got there partly as a result of improved and home-built electronics and partly as a result of my colleague Boris Maiorov's very clever way of backing out the effects of miniscule temperature variations so they didn't mask our results. We could now see the key isotope of plutonium-239 aging, caused by accumulated damage from its own radioactivity, in real time over the course of hours! This meant that the difficulties in attempting to draw conclusions from accelerated aging mixes (with plutonium-238 added) could be worked around. It also meant that we could see the tiniest changes in phase of plutonium-gallium alloys and that we could obtain detailed, quantitative measurements of the thermodynamics, and hence connect our measurements to the material's internal electronic structure and the equation of state that governs its macroscopic behavior.

With these successes, we had become the owners of two condensed-matter physics problems that perfectly fit the Los Alamos mission.

Problem 1: How do plutonium alloys age? We have a deep obligation to understand this; if we don't, how can we be confident in the effectiveness of our weapons? We can't just look at plutonium or look at a nuclear weapon. And we can't test a weapon to see if it still works. Instead, we have to use all relevant science to understand everything that affects nuclear performance. (The fact that plutonium science turns out to be so enthralling in its own right is a tremendous bonus.)

Radiogenic byproducts of plutonium (helium, uranium, and more), radiation damage, and the thermodynamic stability of plutonium-gallium alloys all contribute to the aging process. Each has a knob we can adjust, such as temperature, gallium concentration, and even decay rate by incorporating longer-lived plutonium isotopes. We are now in the middle of this investigation, but already we know some things. Consider, for example, that each radioactive decay of a plutonium-239 atom delivers enough energy to raise about a million plutonium atoms above the melting point. And also consider that the decay constant (the thing that goes in exponentials when one calculates radioactive decays, a little longer than the half-life) for plutonium-239 is about a trillion seconds. Combining these, we expect that in about two weeks, every plutonium atom has been above the melting point, resetting a lot of age-related damage.

So one time scale for aging might be on the order of two weeks, which should be observable if the plutonium is new or the temperature has changed. When we change the temperature to look for this effect, we do indeed see that it takes about two weeks for the system to stabilize to a new, constant, and higher rate of change. Another time scale that we might conjecture would be much longer, based on the decay of plutonium-239 at a rate of 0.003 percent per year. At that rate, in about 350 years, 1 percent of the plutonium-239 is gone, and we can certainly expect to see a 1 percent change in properties. So 350 years might be another time scale (if we somewhat arbitrarily assign significance to the 1-percent level). That one we can't address directly because we can't wait that long, but, surprisingly, what we do see is that the rate of change of the bulk modulus of plutonium after being held at room temperature for about eight years is 0.2 percent per year—about 70 times faster than the decay rate. This rapid rate of change seems to me and my team likely to be caused by the accumulation of material defects from the melting and imperfect re-solidification following each atom's decay.

Problem 2: What is the electronic structure of plutonium, meaning the actual arrangement and behavior of all its electrons? This has been a grand challenge in actinide science for decades. (Plutonium resides in the actinide series of the periodic table.) Constructing such an electronic-structure model would provide deep scientific insight, but would also provide tools to push the equation of state beyond where it can be measured, as well as better models for the thermal conductivity and heat capacity of hot plutonium and maybe even the liquid state—nice to know when making a plutonium casting.

More than two decades ago, my colleague Per Soderlind at Lawrence Livermore National Laboratory suggested that if some sort of magnetic interactions were present, that could explain many of the mysteries of plutonium's electronic structure. But magnetism had never been observed. In fact, a joint paper between the Institute for Transuranium Elements and Los Alamos insisted that there was no magnetism, and that had a chilling effect on what would turn out to be the correct theoretical approaches. However, in 2015, Los Alamos's Marc Janoschek did indeed observe dynamic magnetism using neutron scattering, and a theory was constructed by his co-authors to explain it—including one of the authors of the now infamous paper claiming no magnetism [*see "A Community of Electrons" in the October 2015 issue of* 1663]. However, that theory was based solely on the neutron scattering results and therefore did not address other known properties.

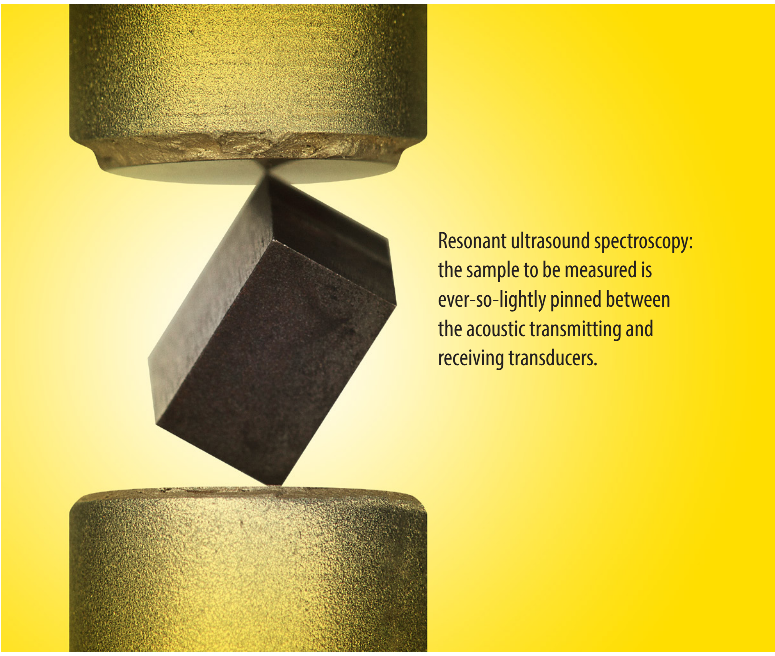
To understand the difficulty plutonium presented to electronic structure theorists, and why this left a big gap, let's examine the thermodynamics of a rubber band. When it is cold, a rubber band has lots of long-chain organic molecules with their bonds lined up in a straight line. When heated, the bond directions vibrate, so that they are no longer lined up. That produces bends in the long chains, making them shorter and thereby producing negative thermal expansion. Unlike a metal, you heat rubber and it gets smaller. That's a general result, in the sense that to fight against the more probable outcome of an expanded solid (entropy benefit), there must exist a thermally accessible state that has a smaller volume when warm. This works for Invar, a zero-expansion iron alloy, and for more exotic materials like zirconium tungstate, where vibrating oxygen octahedra act just like the molecules in rubber.

However, our work on delta plutonium alloys with zero thermal expansion showed elastic softening upon warming that was an order of magnitude greater than that for, say, aluminum, which has a similar melting point. The trouble is,

WE ARE NOW SITTING ON TWO BREAKTHROUGH THEORIES, ONE OF WHICH COULD FINALLY EXPLAIN PLUTONIUM'S ELECTRONIC STRUCTURE.

usually the higher-energy, smaller-volume state that blocks thermal expansion is stiffer, not softer (think of something being compressed). But Per and I realized right away that we could use his previously discredited model (the "Soderlind model"), the known thermal expansion (or lack thereof), and the energy value of Janoschek's dynamic magnetism to compute the neutron scattering results, volume, and stiffness versus temperature.

We had no idea what the calculation would produce. If it made warmer delta plutonium stiffer, then it would be wrong. So we closed our eyes, hit enter on the computer, and waited



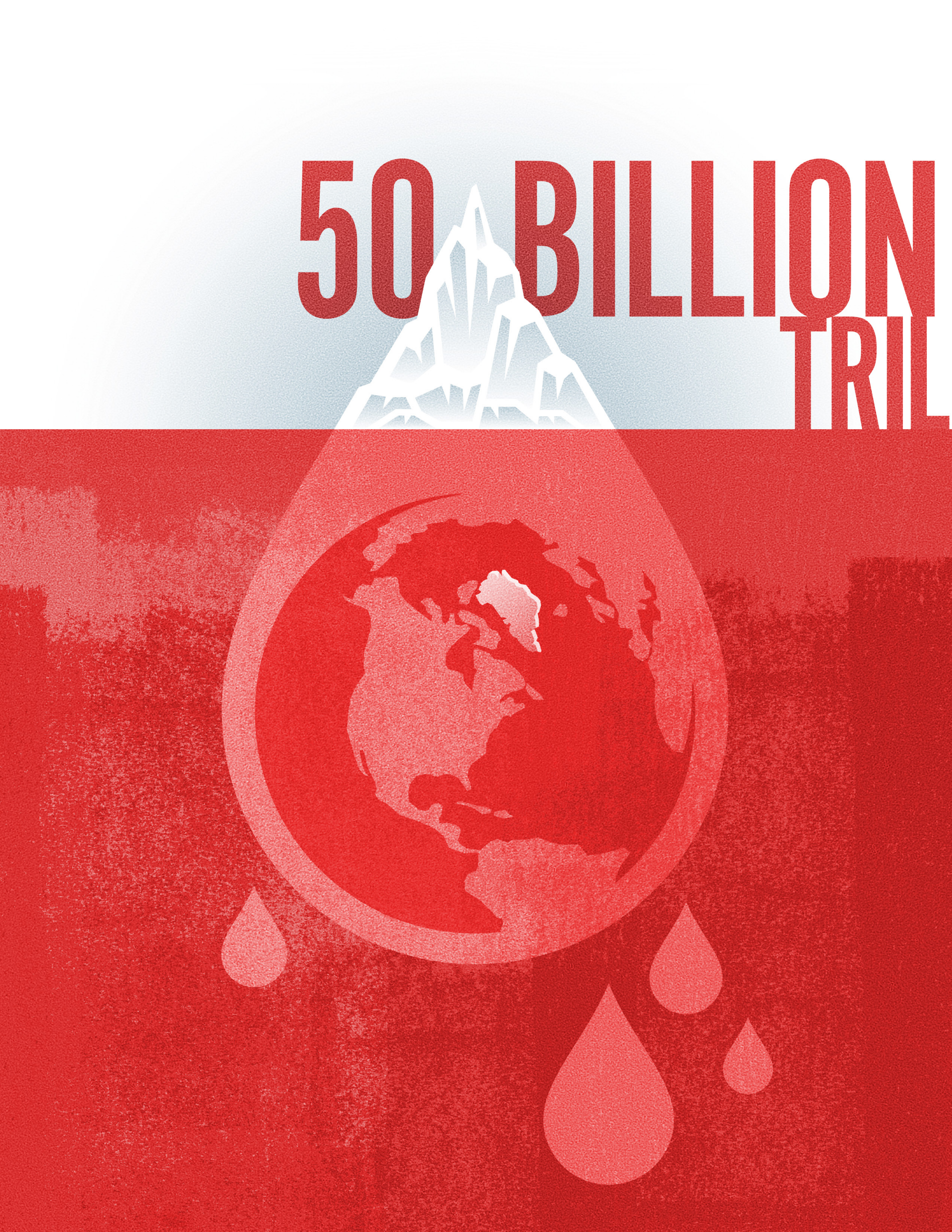
Resonant ultrasound spectroscopy: the sample to be measured is ever-so-lightly pinned between the acoustic transmitting and receiving transducers.

for the massive computation to proceed. Well, something like that. And what we saw made us very happy. The calculation predicted a softening of delta plutonium with absolutely zero volume change, which is indeed what actually happens.

And we are now sitting on a breakthrough in the understanding of the fundamental electronic structure of plutonium. We have two theories in less than a year, constructed once the awful bottleneck of no plutonium magnetism was removed, with both Los Alamos and Lawrence Livermore involved. One theory gets several effects qualitatively correct, the other only applies to one measurement, but both are plausible. And those theories predict several other measurables, including the all-important Fermi surface—the state of the highest-energy electrons in the material, which can only be measured at the Los Alamos National High Magnetic Field Laboratory—as well as some magnetic and thermodynamic properties. Plutonium hasn't been this exciting in a long time, with the promise of clear, hypothesis-driven measurements directed at validation of two new theories, one of which could finally explain plutonium's electronic structure.

So, unlike my first few days at Los Alamos 43 years ago, I can see now many fascinating questions in physics, with answers essential to the Laboratory mission and to national security and with progress only possible in the team environment of a national lab. I am immensely privileged to be able to ask world-class scientists about things that confuse me and receive patient responses. I look back at successes in measurement science, plutonium, materials science, chemistry, and more. And I realize that I am addicted to the visceral reaction, rare and precious, of discovering something that until that moment, no one on the entire planet knew.

I'll bet there's a lot more to come. LDRD


50 BILLION
TRIL

Greenland was once lush green tundra and will be so again as its melting ice sheet submerges the world's coastlines. (And, by the way, Antarctica's ice sheet is nearly ten times bigger.)

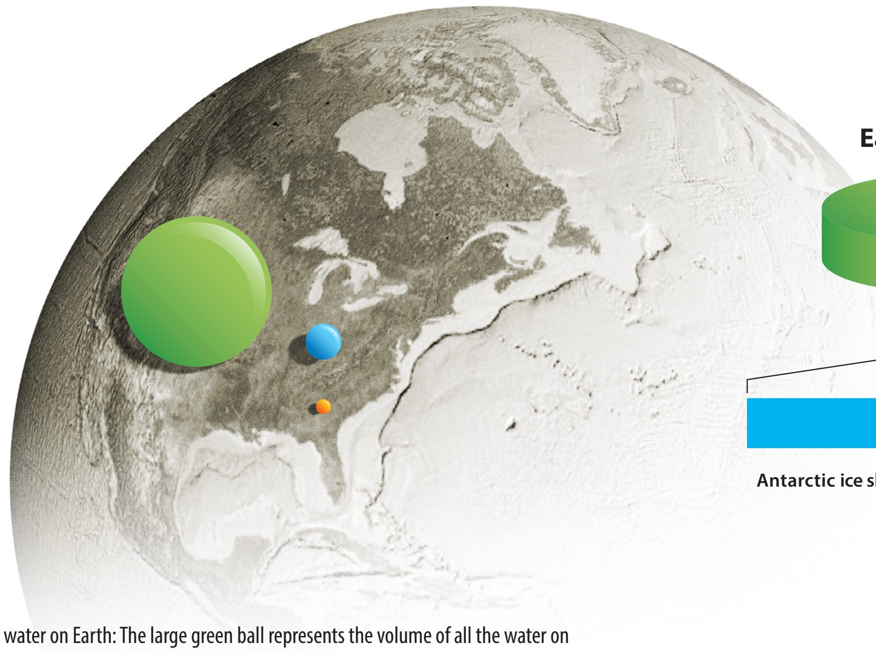
LION DROPS IN THE OCEAN

THIS IS GOING TO SOUND LIKE THE NOW-FAMILIAR STORY about humanity's reckless abuse of the earth and the grave consequences it will have. The story begins with what everybody already knows, that the world is warming, and things are changing in dramatic ways, from droughts to floods to fires to extinctions and, at issue here, rising seas. But this is only barely one of those "unless we do something about it soon" stories. Because while an extremely rapid and comprehensive shift in the world's energy policies could still prevent the worst of it—as predicted in a handful of "let's all adopt renewable energy and buy a Tesla right now" scenarios, as Los Alamos climate scientist Jeremy Fyke calls them—the overwhelming majority of realistic scenarios will result in tremendous ice-sheet loss and sea-level rise.

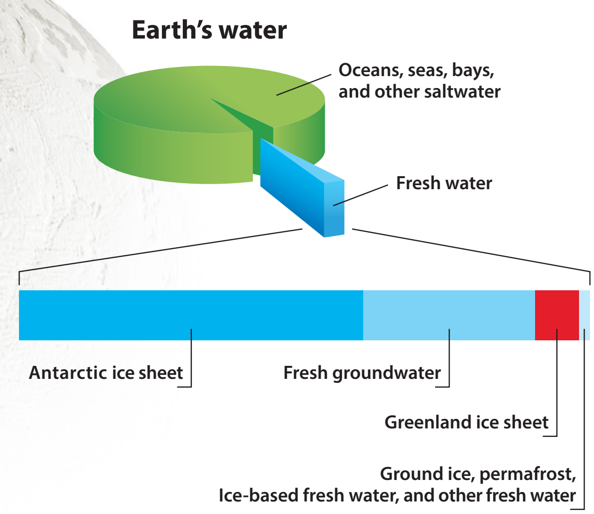
Fyke tracked a wide range of possible carbon-emission scenarios and their corresponding climate trajectories, and with very few exceptions, they consistently agree about one thing. The massive Greenland ice sheet—accounting for about 8 percent of all the world's fresh water and measuring longer from north to south than the continental United States—will melt into the ocean. The process could take thousands of years, but sometime this century, the human race is expected to make the vast majority of this melt inevitable.

Two ice sheets

In the 1995 movie *Waterworld,* Kevin Costner inhabits a future Earth almost entirely covered in ocean. Realistic? Not to that extreme. There isn't enough water on Earth in any form to submerge that much land. Nonetheless, loss of the Greenland ice sheet would push sea level more than 20 feet higher. That's enough to submerge all or part of virtually every coastal city in the world, plus huge swaths of low-lying land in places like Bangladesh, the Netherlands, the American Gulf Coast, and many others. Florida, for instance, would be a dramatically smaller state. And London, more than 35 miles from the nearest sea, would be under water.



All the water on Earth: The large green ball represents the volume of all the water on the planet, if it were pulled from the oceans, ground, and atmosphere. Only 3 percent is fresh water (blue), with about two-thirds of that stored in the Antarctic and Greenland ice sheets, split roughly 90–10 between them. The small orange ball represents all the fresh water accessible for human use, such as groundwater, lakes, and rivers.
Illustration credit: Jack Cook ©Woods Hole Oceanographic Institution



CREDIT: USGS, NSIDC, NASA

Then there's the Antarctic ice sheet to consider. It is nearly ten times larger than Greenland's, and if it were to disappear entirely (a big "if"), that would add another 190 feet of sea-level rise. It goes without saying that the world's coastal cities, in their present locations, would be completely destroyed. Beyond that, the continents would be a lot smaller, with considerably less available land—except in Greenland and Antarctica themselves. Major river deltas, such as the Amazon, Mekong, and Mississippi, would see Great Lake-sized swaths of land completely gone. In numerous regions around the world, interior lands would become coastal; coastal peaks would become islands; and islands would become nothing.

All of this has already begun. According to NASA, the global mean sea level has risen nearly 20 cm (8 inches) since 1870 and is accelerating, having gained almost 9 cm (3.5 inches) just since satellite-based data collection started in 1993. And even though today melting in Greenland and Antarctica together contribute only about a millimeter to sea-level rise each year (plus a few more millimeters from other sources), the future trajectory under business-as-usual carbon emission scenarios is clear: a reversion to an ancient world at a pace unprecedented in the earth's natural history.

"Under a business-as-usual emissions scenario, we're talking about a return to the Cretaceous, like with trees on Antarctica," Fyke says. "And it will stay that way for a long time." That is because it is a lot harder to rebuild the ice sheets than to melt them in the first place. In large sections of Greenland, for example, ice piled higher than 10,000 feet will melt away, lowering the surface elevation to the level of the underlying bedrock, which is close to sea level for much of the enormous island's interior. With that reduced elevation comes warmer weather, causing precipitation to fall as rain instead of snow that might otherwise rebuild the ice sheet. In other words, average global temperatures may have to drop—not just back to preindustrial levels, but substantially *below* them to ice-age levels—for ice sheets to reappear and bring the global sea level back down.

The ice sheets of Greenland and Antarctica are two very different beasts. In Greenland, ice loss comes primarily from glacial flow and surface melting: some ice flows directly into the ocean, where it melts or forms icebergs, while other ice melts on the surface and then flows as water to the ocean. Antarctica, on the other hand, is isolated from the rest of the world by the cold circumpolar Southern Ocean, making it considerably colder than Greenland and thereby preventing significant surface melting. In addition, much of the Antarctic glacial ice extends great distances over water, rather than breaking off upon leaving the land. Such marine ice shelves, warmed by direct contact with the underlying sea, are the primary locations for Antarctic ice loss. In other words, while Greenland is melting primarily because the air is getting warmer, Antarctica is melting primarily because the ocean is getting warmer. The physics of the two processes is quite different, with Greenland's process considerably better understood at present—in no small part because, as Fyke says, accessing sub-shelf cavities in Antarctica is "nearly as difficult as sending a spaceship to another planet."

PLANET EARTH IS GOING TO HAVE LARGER OCEANS AND SMALLER CONTINENTS

Much of Fyke's recent work has focused on Greenland, which is currently losing ice about twice as fast as Antarctica. Most of Fyke's colleagues at Los Alamos, however, are turning their attention to improving models of Antarctica. It's much harder work because there are bigger unknowns with Antarctica than there are with Greenland. But there's also a lot more ice to worry about, so those unknowns translate into much greater uncertainty in future sea-level rise.

Melting ice and boiling beaches

Fyke and his colleagues use sophisticated computer simulations to study the coupling between ice sheets and climate, as is necessary to correctly capture the effect each has on the other. Warmer air leads to smaller ice sheets, certainly, but conversely, when a gigantic mountain of ice goes away, global air-circulation patterns change in ways that can't be ignored. Without such couplings properly taken into account, climate model predictions go increasingly awry as they project further into the future.

"There's a tremendous amount of inertia in the coupled climate system," Fyke says. "Due to feedbacks, in certain cases it's like a ball kicked over the lip of a hill. Once it is sufficiently set in motion, it will continue rolling for a long time." And therein lies the crux of the issue that occupies so much of Fyke's professional attention. Since rapidly accumulating carbon emissions over the coming decades will determine the long-term temperature for many thousands of years to come—and since ice sheets lose elevation more easily than they regain it—how long will it be until the Greenland ice sheet, already melting rapidly, reaches a point of no return? Using an established middle-of-the-road emissions scenario (which humanity is significantly outpacing so far), he estimates that in about 50 years or less, cumulative carbon emissions will drive the ice sheet to a point of no return for long-term deglaciation towards a nearly ice-free state.

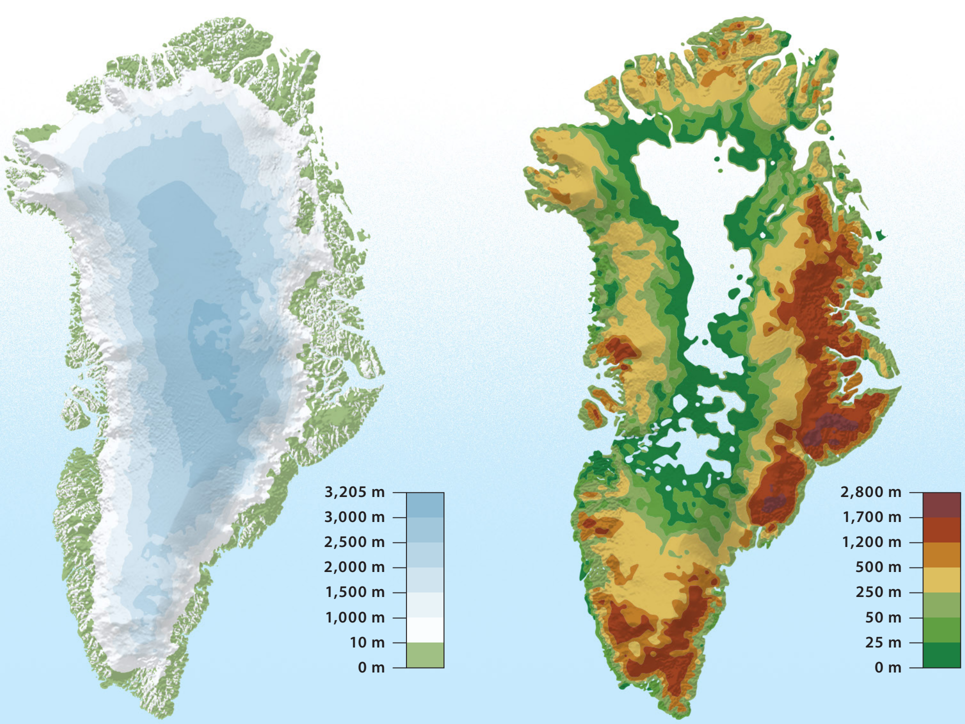
This is an extraordinarily impactful near-term threshold, to be sure, but melting ice is hardly the only far-reaching planetary change looming on the horizon. For instance, farther down the cumulative-emissions road lies a different kind of threshold—not for polar ice sheets or coastal cities, but for human survivability on tropical lands. A cutoff value of something known as the wet-bulb temperature, which blends normal temperature and humidity, marks the highest temperature that mammal physiology can handle by evaporative cooling, such as sweating. Above that wet-bulb temperature, humans and other mammals—even naked, in the shade, in front of a fan—gain more heat from the air than they lose and ultimately experience fatal overheating.

WE COULD BE GOING BACK TO THE CRETACEOUS—IMAGINE ANTARCTICA WITH TREES

Climate models predict that within a few hundred years of ongoing business-as-usual emissions, the wet-bulb temperature throughout much of the tropics will be too high to support human life. Clear limits on how much heat and humidity mammals can tolerate—"probably from experiments on thousands of rats," Fyke says—indicate that people exposed to those conditions would overheat and die from heat stress, rendering much, and perhaps most, of the tropics (in addition to the submerged coastlines) literally uninhabitable.

It's the money

Fyke doesn't just work with complicated and computationally demanding climate models. He has also designed an energy-economy model that calculates rates of fossil-fuel discovery, extraction, and consumption based on a large number of factors that change over time. These factors include, for example, population growth and average per-capita energy use, the relative prices of fossil and non-fossil energy, and the



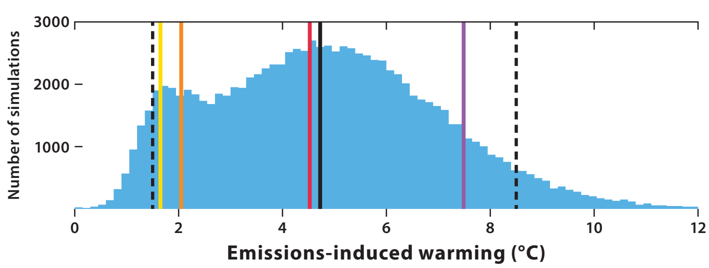
Greenland's ice sheet covers more than 80 percent of the island and reaches a maximum thickness of 3200 meters (10,500 feet). The current elevation profile of the underlying bedrock suggests that upon complete melting, Greenland would accommodate a large inland sea, similar to the Mediterranean. However, most or all of this land would rise above sea level without the weight of the overlying ice sheet.
CREDIT: (left) Eric Gaba, (right) NOAA

rate at which society transitions to non-fossil energy once its price dips below that of fossil energy. (This latter transition will be gradual because existing fossil-fuel infrastructure cannot be replaced with non-fossil infrastructure overnight.)

Ultimately, the model predicts cumulative carbon emissions, and a critical part of the analysis involves the key factors that affect the relative pricing of fossil and non-fossil energy. For example, how large are the world's existing, easily accessible fossil-fuel reserves? What carbon tax might be applied to fossil energy use? How rapidly will non-fossil resources drop in price with economies of scale as they are more widely deployed? How long will it take to shift to non-fossil energy sources once the two prices reach parity?

For each of these and other uncertain parameters in Fyke's model, based on expert opinion where available, he assigns a range of possible values and an accompanying probability distribution using a standard bell curve, or "normal distribution," to capture the greater likelihood of central values but also the possibility of extreme values. In total, he combines 17 such parameter distributions. Because the parameters are probabilistic, each is chosen randomly in accordance with the specified probability distributions in a way that varies from one simulation to the next and, when taken together, describes a wide swath of possible future scenarios.

Once less than 5 percent of total energy demand in any given run of the simulation is found to be supplied by fossil-fuel sources, which Fyke considers a sufficiently complete transition to non-fossil energies, he tallies the cumulative carbon emitted by that time. He feeds that figure into a mathematical relationship known as the Transient Climate Response to Emissions (TCRE), which relates cumulative carbon emissions to the resulting global average rise in surface temperature that is reached—and largely maintained for centuries after all carbon emissions have stopped. The TCRE relationship, remarkably simple in its linearity, was discovered recently by climate scientists using complex numerical carbon-cycle–climate models. It is derived from simulations performed at various climate-modeling centers



Of 100,000 supercomputer runs of a coupled ice and climate simulation using a probabilistic evaluation of 17 key unknown parameters—such as remaining fossil fuel resources, any future carbon tax, and the rate at which non-fossil-fuel energy prices drop over time—global temperature peaks between 1.4 and 8.5°C above preindustrial levels (dashed lines, indicating the 5th and 95th percentile results). The mean rise is 4.7°C (solid black line). Approximate threshold values for key climate tipping points are shown with colored lines: loss of the Greenland ice sheet (yellow), 2°C standard target level (orange), loss of additional carbon-dioxide uptake by vegetation (red), and heat stress rendering tropical regions uninhabitable to humans and other mammals (purple).

and is itself a source of uncertainty, carrying with it another probability distribution in Fyke's analysis.

Importantly, several poorly understood climate processes, such as the release of methane (a powerful greenhouse gas) from thawing permafrost, are not yet included in the simulations that generated the TCRE. As a result, the range of values that describe the warming response to carbon emissions in Fyke's work is potentially too low. These omissions mean that his results are probably a conservative lower bound on actual temperature change in response to emissions.

Despite the significant uncertainties, Fyke was able to validate his simulation with a hind-cast. He set it to start in 1980, using parameter values and probability distributions appropriate to what was known then, and allowed it to predict energy consumption and carbon emissions from that point until 2012, a time period with good data for comparison. Then, upon demonstrating success with past data, he set simulations to predict forward into the future.

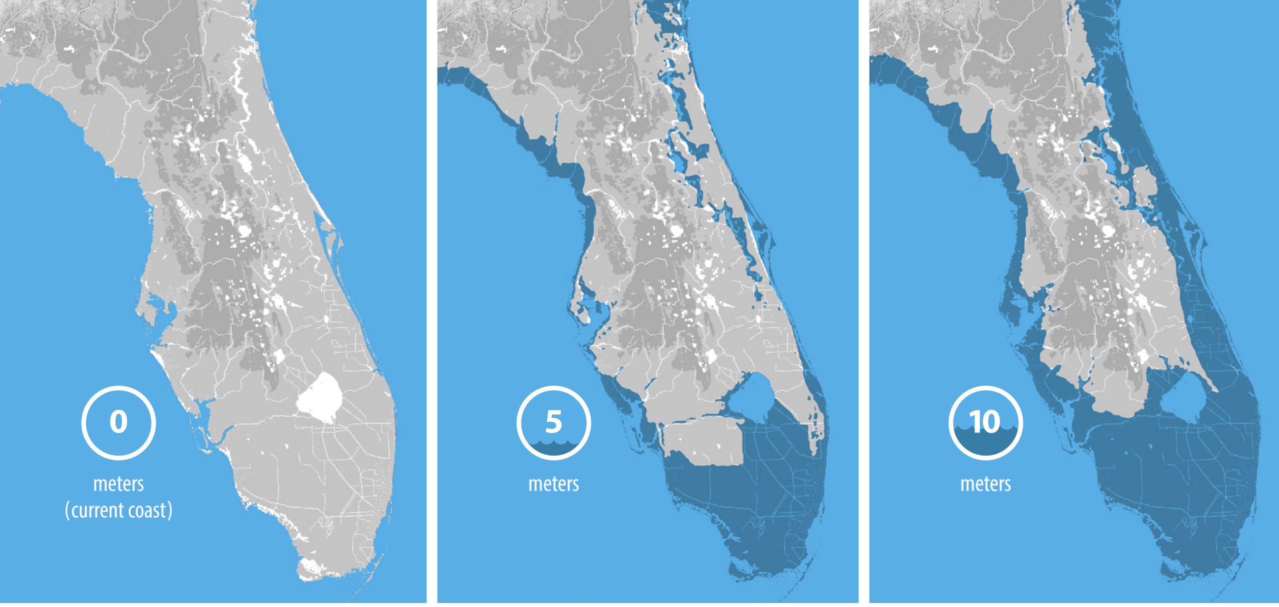
Bad news first

To fully explore all possible future scenarios, Fyke ran 100,000 forward-predictive simulations. Each run yielded a different outcome due to the inherently probabilistic nature of the experiment, but with so many runs, a coherent picture emerged to reveal which planetary warming outcomes are most likely. In fact, the likelihood of a given level of temperature rise could be measured by how many runs within the ensemble produced that result.

THE MODEL IS CONSERVATIVE, MEANING THE REAL RESULTS COULD BE MORE EXTREME

In the average result across the full distribution of simulation outcomes, the global surface temperature increase due to human-induced climate change—already at 0.9°C (1.6°F)—is slated to peak at 4.7°C (8.5°F). That's well beyond several key climate thresholds, such as the oft-quoted allowable limit for temperature rise of 2°C, at which scientists predict extreme and widespread wildfires, crop failures, droughts, and heat waves, with the hottest days of the year in much of North America, including New York and Washington, D.C., as much as 8°C (14°F) hotter than before. At about 4.5°C, global vegetation is expected to max out its ability to soak up additional carbon dioxide from the atmosphere. And what about the calculated threshold for the stability of the Greenland ice sheet and the 20-plus feet of sea-level rise it's currently holding back? That's only 1.6°C. Only about 6 percent of Fyke's simulation outcomes remain below this level; the other 94 percent all cross it.

The threshold for making many tropical regions uninhabitable to humans and other mammals is estimated to be 7.5°C. About 12 percent of Fyke's simulations cross this temperature



Within the United States, Florida and the Gulf Coast are particularly vulnerable to sea-level rise. This sequence shows much of Florida as it is today (left) and as it will be after a sea-level rise of 5 meters (16 feet, or about 70 percent of the Greenland ice sheet, center) and 10 meters (33 feet, representing all of Greenland and much of Western Antarctica, right). Even just a little over half a meter (2 feet) of water would submerge much of Miami and the South Coast of the state.
CREDIT: Climate Central

threshold. However, as with many climate thresholds, this one is fuzzy; before the world hits 7.5°C, some isolated parts of the tropics will likely have already passed the wet-bulb temperature threshold for habitability.

The silver lining of Fyke's study, depending on one's point of view, comes from the fact that it targets no particular public policy initiative or intergovernmental collaboration to curb emissions. Rather, it is intended to simulate all possibilities, all the way from a continuation of the previous century's reliance on fossil energy to a rapid transition to a clean-energy world. The huge range of climate responses the model produces under these diverse scenarios clearly demonstrates that if governments, businesses, and citizens wanted to, they could greatly influence the range of future warming. For example, they could almost certainly save the tropics from lethal warmth and maybe even come in below the 2°C cutoff. Saving the Greenland ice sheet remains a stretch, as a significant part of it melting and raising sea levels seems all but inevitable based on Fyke's simulations. But preventing other undesirable outcomes remains possible, and the simulation results even reveal how to go about it.

"We performed a multiple linear regression of normalized input parameters and were able to identify which policy levers make the most difference in heading off climate change in the model," says Fyke. He notes that the biggest factor within human control turns out to be the price of non-fossil energy. "If governments subsidized non-fossil energy—or conversely, increasingly taxed carbon emissions in a politically acceptable and revenue-neutral way—they could ensure we stay on the lower end of the range of possible warming outcomes." Other climate policy researchers using completely different methods have similarly concluded that such subsidies or taxes would provide an efficient mechanism for minimizing future climate change—providing useful corroboration for Fyke's novel model.

Keep calm and paddle on

All evidence from Fyke's research indicates that government, private sector, and societal action to mitigate climate change would have to be sweeping to save much of the Greenland ice sheet, because its cumulative carbon-based tipping point is so close. And if most or all of Greenland goes, a comparable volume (or more) from Antarctica could add its meltwater to the ocean as well. That means the likely outcome in the centuries and millennia to come, Fyke concludes, is a greatly changed world: huge swaths of coastal land lost, huge swaths of Greenland and other arctic regions made temperate and accessible, and a wide basket of fundamental changes and challenges everywhere else. Future generations will live on a very different planet. But in a profound twist, exactly how different will be determined mainly by the current generation.

In the meantime, Fyke and his Los Alamos colleagues are turning their attention to the largest question mark in their coupled ice and climate models, Antarctica. Its ice sheet, ice shelves, saltwater sea ice, and rising Southern ocean temperatures all couple to the broader climate system, sharing numerous complex feedbacks yet to be spelled out in detail. Los Alamos scientists and their supercomputers are working to understand the interplay of changes facing the planet. So the answers are coming, whether or not the solutions are.

—Craig Tyler

More **climate science** at Los Alamos

- **Climate and ocean modeling**
  http://www.lanl.gov/discover/news-release-archive/2014/September/09.25-climate-earth-system-project.php
  http://www.lanl.gov/newsroom/picture-of-the-week/pic-week-9.php
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  http://www.lanl.gov/discover/news-stories-archive/2015/March/climate-and-wildfires.php
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LITTLE LASER BIG SCIENCE

A universally useful tool pioneered and perfected at Los Alamos is exploring other planets and improving life on this one.

Mars's Mount Sharp, the source of new geological LIBS data that suggest Mars may have once been flush with both liquid water and atmospheric oxygen.
CREDIT: NASA/JPL/MSSS

SOME TOOLS, LIKE A CROSSHEAD SCREWDRIVER, are only good at the task for which they were invented. Others, however, like a flathead screwdriver, are often useful for tasks beyond their original one. Over 30 years ago, scientists at LosAlamos developed a tool for watershed preservation that detects and measures naturally occurring toxic metals in soil. That tool is now being used in various scientific endeavors, from exploring Mars's chemical makeup to protecting precious pipelines.

Laser-induced breakdown spectroscopy (LIBS) is a technique that reveals the presence and concentration of elements in a sample. A small but powerful laser is used to vaporize a miniscule amount of material from the surface of the sample, creating a tiny plasma that contains energetically excited atoms. As the plasma cools, the atoms emit light at wavelengths characteristic of their elements and a spectrometer measures the light emissions, which are then used to calculate the concentration of each type of atom in the sample. LIBS is handy because it's virtually nondestructive, portable, adaptable, rapid, remote (can measure a sample from a distance), and affordable—which is why it can be used in so many environments, including other worlds.

The latest news from Mars came via ChemCam, a Los Alamos LIBS analyzer aboard the rover *Curiosity*. Deposits of manganese oxide and strong silica enrichment were discovered, suggesting that liquid water may have been present much later, and that there may have been more oxygen in the planet's past, than was previously thought.

"Manganese deposits only formed on Earth after the rise of photosynthesis, when the atmosphere was flooded with free oxygen produced by photosynthetic microbes," explains Los Alamos planetary scientist Nina Lanza. The manganese deposits on Mars suggest that Mars too had significant amounts of oxygen in its atmosphere at some point, although the source of that oxygen is still unclear. One hypothesis is microbes. Another is that the oxygen came from water molecules being split by ionizing radiation, resulting in the lighter hydrogen atoms escaping Mars's atmosphere and the heavier oxygen atoms staying behind.

Laser-induced breakdown spectroscopy, or LIBS, is a technique to reveal what elements are present in a sample. A powerful laser is used in quick, successive pulses to ablate nanograms of material from the sample's surface, creating a micro-plasma in which energetically excited atoms dissociate into ions and electrons. As the excited atoms and ions lose their excess energy, they emit characteristic wavelengths of light, and a spectrometer is used to resolve the wavelengths and measure the intensity of those emissions to determine which elements are present in the sample and in what relative proportions.

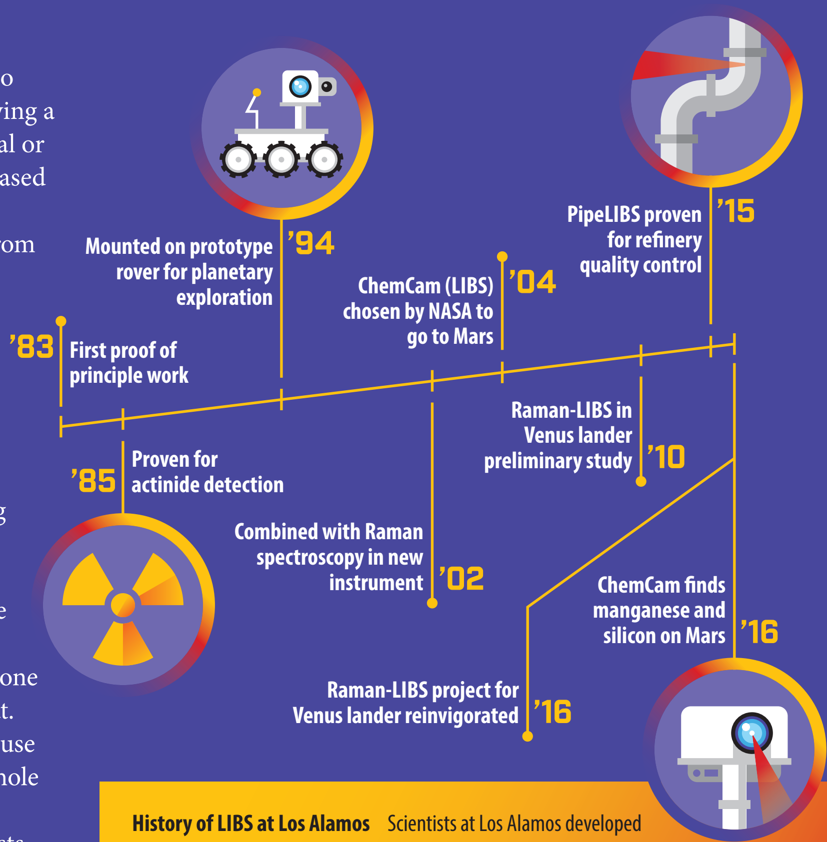
The discovery of rocks strongly enriched with silica led to two more discoveries. First, the detection of tridymite, a silicate mineral that is rare on Earth, was the first-ever evidence of Martian silicic volcanic activity, which is a specific type of explosive volcanism.

"The second discovery," Lanza's colleague astrogeologist Jens Frydenvang explains, "came from where, within Mars's bedrock, we found high-silica. It was along the fractures, which suggests that liquid water was present much later than previously thought—extending the time period in which Mars could have supported microbial life."

As successful as ChemCam has been, Los Alamos scientists are eager for data from the next rover, scheduled to launch in 2020. Its updated Los Alamos instrument dovetails LIBS with Raman spectroscopy, a technique that identifies specific molecules, complementing the elemental analysis of LIBS.

Back here on Earth, LIBS is proving to be quite useful for national security in several arenas. LIBS can be used by International Atomic Energy Agency inspectors to rapidly detect the presence of nuclear material in a variety of samples, with little-to-no sample preparation. Because LIBS can distinguish between different isotopes of the same element, it can be used to determine the composition of enriched uranium oxide samples. It could also be used, if needed, to safely acquire reliable field measurements of debris, following a nuclear event. Some nonnuclear weapons, such as chemical or bioweapons, or even explosives, are also subject to LIBS-based detection and identification.

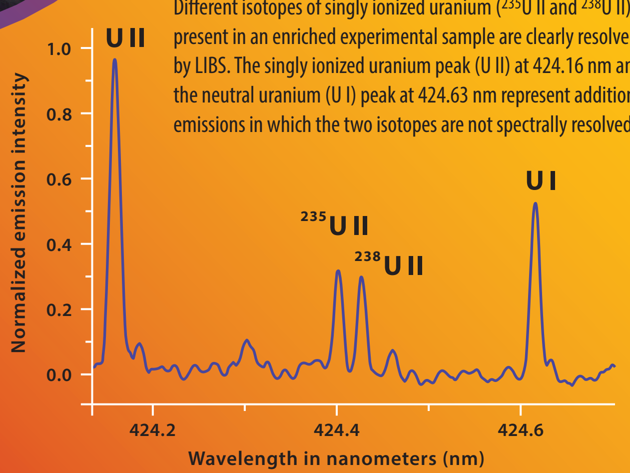
Another security-related application of LIBS comes from the oil industry. Loss of infrastructure, loss of productivity, and even loss of life have occurred in the past when refinery pipes suddenly failed, causing explosions. The steel used to make refinery pipes, which carry corrosive chemicals, needs a minimum concentration of silicon in order to resist corrosion. A backpack-mounted LIBS system called PipeLIBS, developed by Los Alamos scientists James Barefield and Elizabeth Judge, is now being deployed in refineries. It will be used to examine pipes prior to installation and also to inspect existing pipes and identify risks. The walls of refinery pipes carrying corrosive liquids are allowed to be no thinner than one-eighth of an inch. Yet Barefield and Judge have discovered corrosion-prone pipes in service that may have been much thinner than that. PipeLIBS is the only way to check pipes that are already in use because conventional chemical analysis requires cutting a hole in the pipe, which defeats the purpose entirely.



History of LIBS at Los Alamos Scientists at Los Alamos developed LIBS for watershed preservation; however, the tool has become universally useful. A Los Alamos LIBS instrument is already exploring Mars and may one day explore Venus. National security, including weapons, energy, and food security, is improved by this adaptable, portable, and affordable tool.

In agriculture, food- and water-security scientists are also looking at, and looking with, LIBS. Soil concentrations of essential elements like carbon, nitrogen, potassium, and phosphorus are easily measured with LIBS. Nitrogen-containing fertilizers are liberally applied to crop fields, often in extreme overabundance. The plants only take up so much, and the rest ends up contaminating the water table. Judge and Barefield, along with collaborators, are using LIBS to investigate solutions for this nitrogen overdosing: precision agriculture and sustainable agriculture.

James Barefield and Elizabeth Judge use their patent-pending, backpack-mounted PipeLIBS system to evaluate the safety of oil-refinery pipes.



Different isotopes of singly ionized uranium (^{235}U II and ^{238}U II) present in an enriched experimental sample are clearly resolved by LIBS. The singly ionized uranium peak (U II) at 424.16 nm and the neutral uranium (U I) peak at 424.63 nm represent additional emissions in which the two isotopes are not spectrally resolved.

Precision agriculture uses LIBS to measure the carbon, nitrogen, potassium, and phosphorus in soil. The idea is to use these data to ensure application of only the precise amount of fertilizer that will equal the plants' uptake. At present, the soil LIBS system is backpack-based, like PipeLIBS, but the goal is to have a LIBS system mounted on the front of a tractor. The soil's nutrients will be measured as the tractor travels, and a dispenser on the back will distribute the precise amount of each element to bring the whole field to uniform, ideal growing conditions.

Sustainable agriculture uses organic material to build up, or biomodify, the soil over several years to achieve optimal levels of these nutrients, guided by LIBS data. The result is a fertilizer-free field that uses much less water, produces higher yields, does not contaminate the water table, and is entirely self-sustaining.

From rocks on Mars to fields on Earth, LIBS is helping scientists do their jobs with improved speed, safety, and precision. And all of that is just at Los Alamos, where LIBS was pioneered. Scientists around the world are using LIBS for environmental assessment, cultural-heritage preservation, green-energy applications, and even crime-scene forensics.

Not bad for a little small-town laser. LDRD

—Eleanor Hutterer

Driving Sustainability

In the future, city transportation systems will be very different. From sustainably sourced materials to automated vehicles, Los Alamos scientists are helping drive transportation technology toward an ecofriendly future.

When something is old and used up we throw it away. We throw away pens, shoes, and umbrellas; we throw away suitcases, beds, and cars. Wait, cars? Yes, cars. Although we don't actually put a car on the curb for the garbage truck, there's little choice for cars that are old and used up but to be junked.

Some materials, such as metals, get recycled, while others, such as tail lights, can be reused. But after the recyclables have been recycled and the reusables have been reused, what remains gets shredded and interred in landfills. With a typical lifetime of about 200,000 miles, Americans throw away roughly 12 million cars every year. Waste reduction and sustainability are moving fast in other sectors but have some catching up to do when it comes to the automotive industry. From concept to scrapyard, there's plenty of room for improvement in how cars are built that can help extend their lives and reduce their waste. Scientists across Los Alamos National Laboratory are participating in several collaborations and national consortia to work all the angles and build inroads toward a more sustainable future of driving.

The zero-waste movement is gaining traction and infiltrating the mainstream. Cities are running out of places to put trash and running low on materials to make new stuff to replace trash, so many are going green to reduce their refuse. Cities, families, and individuals are joining ranks in reducing landfill contributions incrementally over about 20 years. The end goal is 100 percent waste diversion, where nothing goes to the landfill. Plastic grocery bags and take-out boxes are verboten, recycling is compulsory and broadly inclusive (not just soda cans and newspapers anymore), and some cities even have daily curbside pickup of food scraps for community composting programs. Companies, too, are getting on board, redesigning their products and packaging to minimize waste. The old mantra "reduce, reuse, recycle" now includes "repurpose, reclaim" and in some instances "replace," with respect to using alternate sources and materials that are more sustainable and future-friendly. So, what does that mean for cars?

Sustainability in transportation is a many-faceted challenge. The fossil fuels that power conventional cars are limited in supply, as are some of the materials used in hybrid engines. Cars are made from steel, which is heavy, and heavy things require more fuel to accelerate. However, lighter things are more easily damaged and are therefore frequently repaired or replaced. Many parts are made of plastic, which also draws on the finite supply of oil for its production. And of course, greenhouse gases produced from combusting fossil fuels contribute to climate change and air pollution, while discarded plastic and spilled oil pollute the land and water. Sustainable transportation as a paradigm has the charge of maintaining our present standards of travel—speed, safety, comfort, affordability—while no longer relying on finite resources like oil or causing harm to the environment. That's a tall order but also a necessary one.

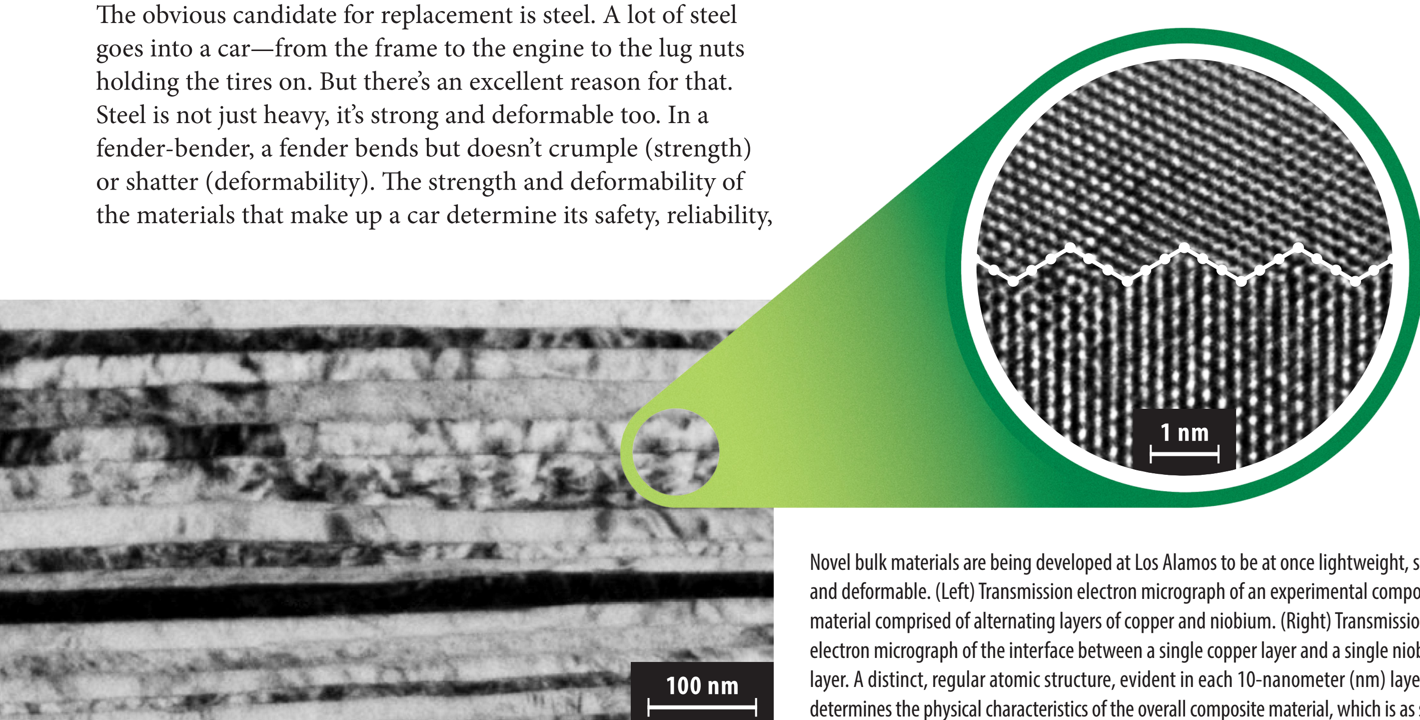
When a car dies, much of its matter gets interred in a landfill.

Lightening the load

One way to reduce a car's environmental footprint is to change what it's made of. For every hundred pounds of weight shed, a car gets a fuel-economy boost of 2 percent. But if a car is too light it will feel like a shoebox on wheels, and it may perform about as well. So it's a matter of finding the sweet spot between the performance and safety of heavier cars and the fuel economy of lighter cars. With this in mind, much effort is going into finding safe ways of lightweighting tomorrow's cars. The obvious candidate for replacement is steel. A lot of steel goes into a car—from the frame to the engine to the lug nuts holding the tires on. But there's an excellent reason for that. Steel is not just heavy, it's strong and deformable too. In a fender-bender, a fender bends but doesn't crumple (strength) or shatter (deformability). The strength and deformability of the materials that make up a car determine its safety, reliability, and performance. So materials with strength and deformability like steel that weigh less than steel would be ideal. But lightweight, high-performance materials like titanium and carbon fiber are expensive. Race car drivers or custom car builders may be willing to pay for these luxury materials to improve the performance of their vehicles, but average American car buyers are not.

Aluminum is being used by major car companies to replace steel wherever possible. Some perks of using aluminum are that it's much lighter than steel, it has high deformability, and the technology and infrastructure for aluminum recycling is well established. But aluminum has some problems too. It's not very strong, and it can be difficult to join pieces together. Welding aluminum is tricky for a number of reasons, including its low melting point, its propensity to harbor impurities, and the fact that aluminum alloys can only be welded to like alloys. Aluminum is also energy intensive to machine or cast, and high heat can weaken it, sometimes forcing manufacturers to resort to using rivets or adhesives to join pieces together.

Magnesium is another metal that is receiving a lot of attention for lightweighting cars. Magnesium has properties that are similar to those of aluminum, but it is 33 percent lighter, easier and less energy intensive to machine or cast, and can be more corrosion-resistant than aluminum. And like aluminum, magnesium has some problems; chief among them are its limited strength and formability and its high flammability. So while magnesium might work for, say, the rims of a tire, it might not be a good choice for the chassis.



Novel bulk materials are being developed at Los Alamos to be at once lightweight, strong, and deformable. (Left) Transmission electron micrograph of an experimental composite material comprised of alternating layers of copper and niobium. (Right) Transmission electron micrograph of the interface between a single copper layer and a single niobium layer. A distinct, regular atomic structure, evident in each 10-nanometer (nm) layer, determines the physical characteristics of the overall composite material, which is as strong as tool steel, despite being comprised of two relatively soft metals.

CREDIT: Materials Today, 16:11, pp 443-449

But maybe the best lightweighting solution can't be found in any extant metal. Maybe it lies in brand new materials. Researchers at Los Alamos's Center for Integrated Nano-Technologies (CINT) are working on creating materials that embody all of the desired features, being at once lightweight, strong, deformable, and environmentally friendly. For example, they've developed a composite material comprised of alternating layers of copper and niobium. Both are soft metals, so they're easy to work with, and they don't mix chemically, so the layers, despite being only 20 atoms thick, remain discrete. This is key because the material as a whole will draw its properties from atomic interactions at the interfaces of the layers, so the layers need to be controlled at a very fine level. The result is a composite that possesses strength comparable to that of the steel used for high-quality hand tools, even though it is constructed of two soft materials. This particular material is too expensive to be a steel replacement itself, but CINT scientists are using it to understand the physical interactions that give materials their strength.

"We're making materials that are ten times stronger than what is commonly available," explains Los Alamos scientist Nathan Mara. "But the big issue is that the manufacture of these materials is centered around the microelectronics industry, which requires thin films. For the automotive industry we need to make much larger sheets, rods, and tubes, which requires a novel manufacturing method." Through a process similar to the ancient technique used to produce Damascus steel for swords (repeated folding and flattening), Mara and others at CINT can produce pieces of the copper-niobium composite metal about the size of a ski. While it's not exactly a sedan side panel, it's the bulk production that's important, and they've just about got that down.

Another material being developed at CINT is comprised of nanometers-thin layers of aluminum and titanium nitride, a strong but brittle ceramic. The metal-ceramic composite material is lightweight and has the best properties of each of its components: the high deformability of aluminum and the strength of titanium. However, it could just as easily have been the worst of both worlds: a weak and brittle material. The way they decide which materials to actually synthesize is through extensive modeling. By looking at the physical characteristics of component materials, like deformability, crystal structure, and stiffness, a computer model can predict what sort of behavior a composite material might exhibit. So far, the models have been right and have led the scientists to some promising new materials.

Extensive integrative modeling also goes into understanding how to maximize a material's performance through the manipulation of its geometry and microstructure. Vehicle lightweighting isn't only about the composition of materials; it also has to do with their configuration. For example, using thicker cross sections of lightweight materials can increase their strength, while thinner cross sections of very strong materials can reduce their weight. Scientists at Los Alamos are developing and characterizing advanced high-strength steels that can do the same duty as conventional materials but with thinner cross sections and different geometries, aiding in keeping weight down while maximizing performance.

Los Alamos National Laboratory is one of ten national labs participating in a new federal initiative to lightweight America's cars: the Lightweight Materials National Laboratory Consortium, or LightMAT, is part of the U.S. Department of Energy's (DOE) Clean Energy Manufacturing Initiative and is funded by the Office of Energy Efficiency & Renewable Energy (EERE). The goal of the Clean Energy Manufacturing Initiative is to boost the productivity and competitiveness of U.S. clean energy technologies in the world market. To that end, the mission of LightMAT is to enable the automotive industry to use some of the unique scientific and technical resources related to lightweight materials that exist within the national labs.

Los Alamos's Ellen Cerreta is on the LightMAT steering committee. She explains how it will work: "LightMAT offers a catalogue of capabilities that come from research and development at our national laboratories. These capabilities can be applied to challenges associated with lightweighting and will facilitate the inclusion of lightweight materials in automobiles. Through this catalogue, the automotive industry can directly access these capabilities to address their specific research needs." The immediate focus will be cars and trucks, but because the technologies are broadly transferable, buses, trains, boats, and planes will also be losing some weight in the near future.

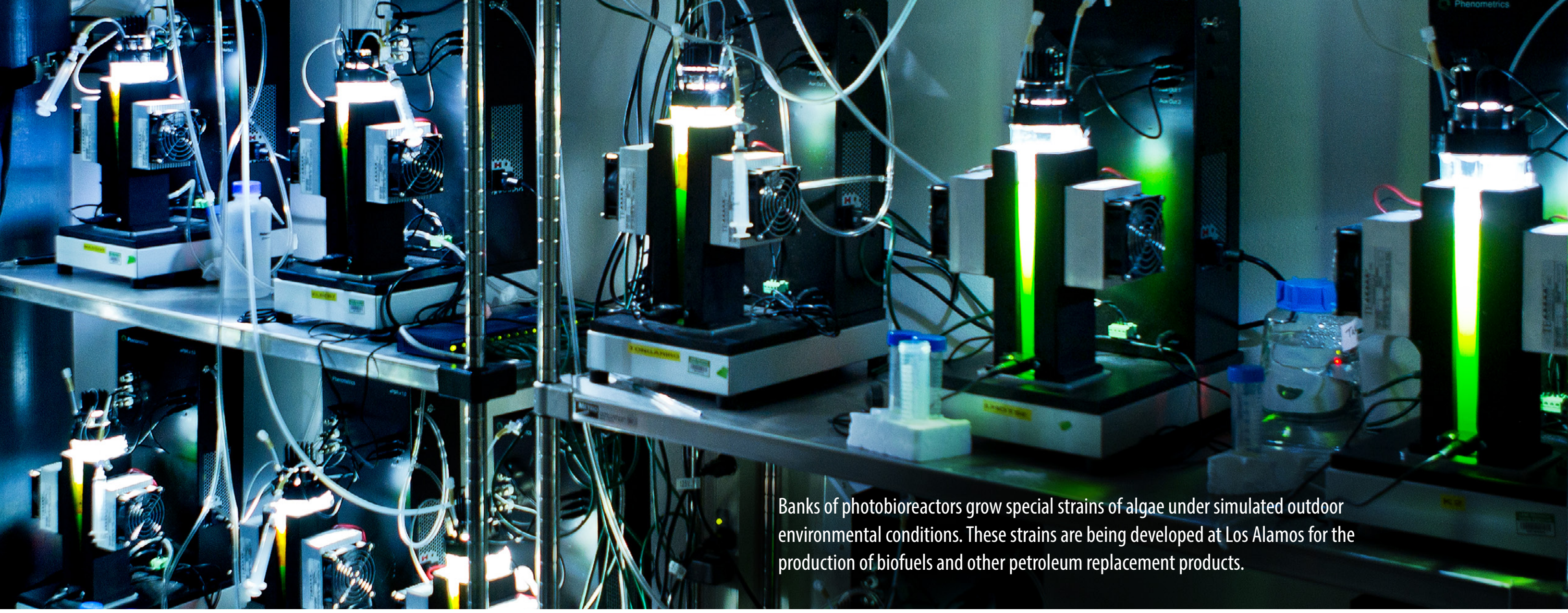
Just one word

Plastics.

What about plastics? Each year, cars contain less metal and more plastic, so it would seem plastics need to get green too. Technically speaking, plastics are a group of malleable, moldable materials that contain synthetic or semisynthetic organic compounds usually derived from petrochemicals. Generally speaking, plastics come from oil.

Plastics are great because they are lightweight, strong, deformable, waterproof, versatile, cheap to make, and easy to work with. With all of those advantages, plastics can't be made pariahs simply because they come from oil, but not coming from oil would be even better. Los Alamos bioenergy scientists are working on petroleum replacement products (PRPs),

For every hundred pounds of weight lost, a car's fuel economy gains 2 percent.



Banks of photobioreactors grow special strains of algae under simulated outdoor environmental conditions. These strains are being developed at Los Alamos for the production of biofuels and other petroleum replacement products.

that is, alternate sources for products traditionally made from petroleum, such as nylon, which is used in auto upholstery (among a great many other things).

"The nylon that could be made would not be a new nylon," emphasizes Los Alamos bioscientist Taraka Dale, "it would be made with the same chemicals that come out of a barrel of oil. This nylon would work the same and feel the same in your hand, because it would be the same material. It's the source that would be different."

Nylon comes from adipic acid, which usually comes from oil. But Los Alamos is collaborating with the National Renewable Energy Laboratory (NREL) on ways to get adipic acid and its biological precursor, muconate, from biomass—that is, plant parts available in large quantities that aren't otherwise needed for food. The approach entails breaking down the bonds of the biomass into sugars, which small organisms like bacteria or yeast can take up and metabolize, releasing muconate or adipic acid as a metabolic product. By modifying, inserting, or deleting genes in the bacteria or yeast, the researchers aim to make industrially relevant quantities of these precursors. Once they have adipic acid, the process of making nylon is the same as with adipic acid from crude oil.

Adipic acid is just one example, however. The Los Alamos and NREL team has joined with seven other national labs in a new, collaborative synthetic biology effort called the Agile BioFoundry, funded by the Bioenergy Technologies Office under the EERE. The Agile BioFoundry ultimately plans to make replacement versions of many other kinds of plastic materials that go into a car—things like floor mats, dashboards, sun visors, consoles, door handles, bumpers, hoses, and reservoirs, just to name a few. Even more importantly, the Agile BioFoundry aims to establish a new, generalizable platform that can rapidly design, build, and test new microbial strains and metabolic pathways for making a broad range of PRPs. This platform will help reduce both the cost and time-to-market for these PRPs, enabling the BioFoundry to meet its goal of rapid scale-up while maintaining the economic viability and sustainability that are central to its vision. Though other communities will almost certainly be interested in the Agile BioFoundry's concept for PRPs, its initial focus will be transportation.

Building a lighter, greener car is paramount to sustainable transportation. But that's just half of the equation; the other half is fixing the fuel problem. Fuel cells are the transportation fuel of the future, but in the meantime, fossil-free fuels are being developed to work in the cars of today. Algae is a promising form of biomass that can be used for fuel and PRP-coproduct production, and Los Alamos has built up considerable expertise in manipulating algae strains in an effort to make fuel precursor molecules in large enough quantities to be economically viable.

Plastics are too good to be made pariahs simply because they come from oil.

Algae produce more oil per land area than other oil-producing plants (palm, soy, safflower, etc.) and can grow on marginal lands in marginal water, making them ideal candidates for a renewable source of energy-dense liquid fuel. Recent algae achievements at Los Alamos include increasing growth rate, increasing oil content, broadening the potential for coproduct production, developing energy-conserving harvesting techniques, and sequencing the genomes of several new potential algae production strains. [*To learn more about algal biofuels at Los Alamos, see "Seeing Green: Squeezing Power from Pond Scum" in the January 2012 issue of* 1663.]

Fuel cell ins and outs

Fuel cells have been around for more than 150 years. They come in several varieties and have been developed for diverse purposes. The space shuttles got electricity in part from fuel cells, as did the Gemini and Apollo spacecraft of the 1960s and 1970s. In the late 1970s, Los Alamos began its program for polymer electrolyte membrane fuel cells, or PEM fuel cells, and the program is now one of the Laboratory's longest-running programs. (Alternatively, PEM stands for proton exchange membrane, but both names refer to the same device.) PEM fuel cells are the most promising for cars, and most major car companies have their own PEM fuel-cell programs. There is little doubt that this technology will power our cars in the future.

A fuel cell is similar to a battery—both devices employ two electrodes (anode and cathode) to use the energy in chemical bonds to drive electrons through an external circuit, creating the electricity that powers a device. A battery contains a limited quantity of chemical reactants to supply electrons, and when the charge stored in those reactants is used up, the battery is discharged. On the other hand, fuel-cell electrodes do not store any charge and can produce power as long as reactants are supplied to the fuel cell, which is limited only by the size of the fuel tank. Fuel cells typically use hydrogen as fuel, which can be made from renewable resources, resulting in electricity being produced with water as the only emission. Moreover, the refueling time and range of a fuel-cell vehicle is comparable to that of a gasoline vehicle.

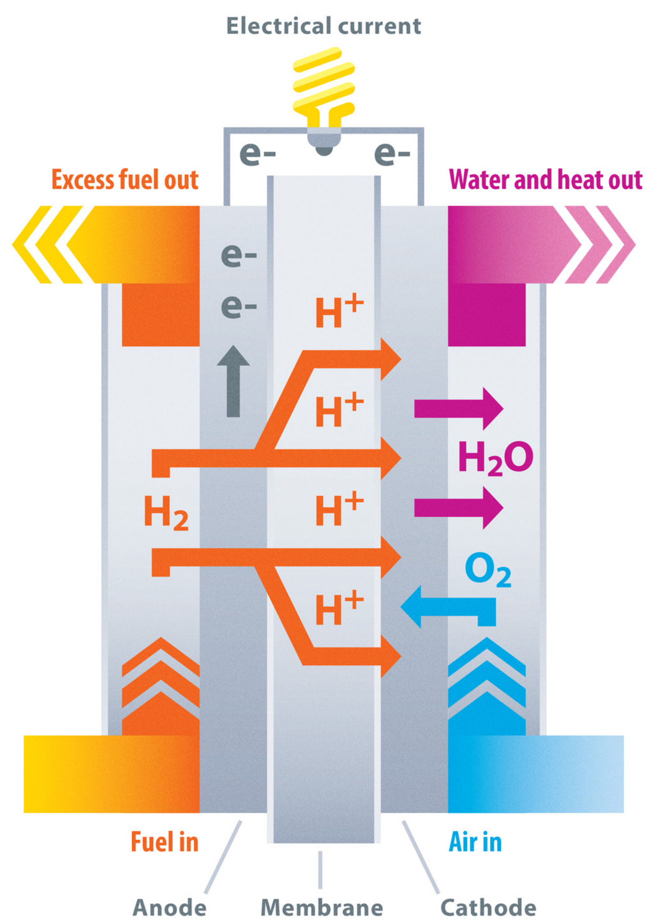
In a PEM fuel cell, hydrogen atoms enter the anode side of the cell and are dissociated with the help of a catalyst into negatively charged electrons and positively charged hydrogen ions (protons). The protons pass easily through a special electrolyte membrane that separates the anode from the cathode. Meanwhile the electrons, which are generated at the anode but can't pass through the membrane, travel along an external circuit, through whatever electrical system the fuel cell is powering, to the cathode side where they rejoin the protons and react with oxygen to produce water. The chemistry is compelling indeed—hydrogen plus oxygen make water, what could be greener than that? But there are still challenges to overcome.

The main fuel-cell challenges at present are cost and durability. One speed bump on the road to sustainability is the cost of certain fuel-cell components. A catalyst is needed on both sides of the fuel cell to facilitate one reaction at the anode and another reaction at the cathode. And as bad luck would have it, the best catalyst by far is one of the most expensive metals in the world: platinum. About 40 percent of the cost of a fuel cell comes from the platinum. Contemporary cars use platinum too—roughly 3–7 grams go into a typical catalytic converter. And while a single fuel cell uses much less than that, once fuel cells start stacking up, as they must to power a car, the quantity of platinum becomes an issue.

The ElectroCat Consortium is a product of the DOE's Energy Materials Network Initiative, in which Los Alamos has partnered with Argonne National Laboratory to get fuel cells past the platinum problem. The quantity of platinum in a fuel cell has to come down in order for fuel-cell technology to be cost-competitive with the internal combustion engine. Platinum is used in both the anode and cathode, but because the cathode contains considerably more, the focus for now is on reducing or replacing platinum there without losing performance or durability. The job that platinum does at the cathode is to split the oxygen molecule to facilitate its combination with the hydrogen ion and electrons to produce water.

Among other ElectroCat efforts, Los Alamos researchers are working on optimizing the production and performance of non-platinum-group metal catalysts. The researchers have developed a methodology that uses nitrogen–transition-metal–carbon catalysts for the electrochemistry on the cathode side. Depending somewhat on which transition metal is used in the catalyst being tested, the researchers can achieve high power output, good efficiency, and promising durability.

One potential way to move away from a platinum catalyst is to operate fuel cells under basic, or alkaline, conditions. Fortuitously, non-platinum-group metal catalysts perform as well, and even better in some cases, than platinum does in an alkaline environment. However the lack of a suitable membrane that has high conductivity and stability under alkaline conditions has hindered the development of these fuel cells. But in a recent DOE Advanced Research Projects Agency-Energy project, a Los Alamos experimental membrane outperformed all its competitors in very alkaline conditions.



Schematic of a polymer electrolyte membrane (PEM) fuel cell. A PEM fuel cell has two sides, each with an electrode (anode and cathode), separated by a polymer electrolyte membrane that keeps the chemistry on the two sides from mixing. The fuel (hydrogen gas) is channeled into the anode side and air (containing oxygen) is channeled into the cathode side.

Another problem plaguing progress is the tendency of the membrane and catalyst materials to degrade under operating conditions. The Fuel Cell Consortium for Performance and Durability (FC-PAD) includes several national labs as well as partners in industry and academia working together to commercialize low-platinum fuel cells. This Los Alamos-led consortium was assembled to address the durability challenge head on.

FC-PAD is evaluating state-of-the-art commercial electrocatalysts under relevant conditions to quantify how well they perform. It's not enough to know under what conditions a material degrades; developers also need to know why and how the degradation occurs. Then commercial catalyst makers can take that data and improve their products accordingly, or operating procedures can be developed to minimize the degradation. In addition to characterizing materials already on the market, FC-PAD scientists are testing pre-commercial products that they are trying to get to market and also conducting fundamental research toward design principles for new materials.

"We know how to make durable fuel cells," says Los Alamos fuel-cell program manager Rod Borup, "but we don't know how to make them at a cost that would enable mass commercialization." FC-PAD is trying to reduce the quantity of expensive materials like platinum by optimizing the fuel cells' structure to increase the performance of the catalyst.

Even beyond the scope of FC-PAD, laboratory scientists are working on a whole new class of PEM fuel cells to improve fuel-cell functionality. The two main types of PEM fuel cells on the market today are low-temperature PEM fuel cells, which work best below 80°C, and high-temperature PEM fuel cells, which work best above 160°C. That leaves a big gap in fuel-cell functionality.

"This is a bad place to have a functionality gap, because this temperature regime can relax certain engineering constraints for fuel cells," explains Andrew Dattelbaum, the Los Alamos Materials Synthesis and Integrated Devices group leader. "So to reduce the overall system costs, we would really like to develop devices that function well in that temperature range." Prototype fuel cells using an experimental new membrane material developed at Los Alamos recently demonstrated excellent performance and durability across a larger temperature range, from 80°C to 200°C, handily filling in this functionality gap.

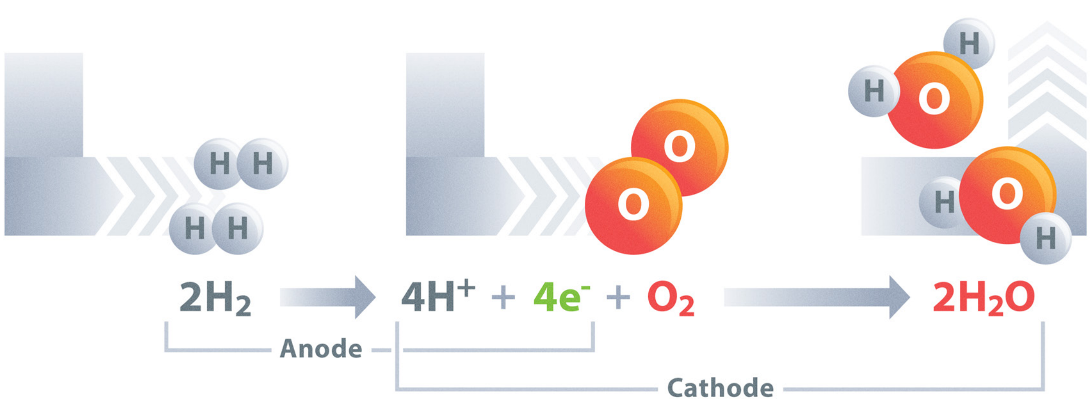
Fuel cells will undoubtedly power our cars in the future.

The final roadblock to consider for fuel-cell vehicles is the fuel-cell fuel itself: hydrogen. Presently, pure hydrogen gas, or H_2, is acquired by steam reforming of methane—reacting methane with steam at high temperature. Methane is a fossil fuel, so as long as the hydrogen in PEM fuel cells comes from methane, the fuel cells aren't completely sustainable. However, the greenhouse-gas emissions associated with steam reforming of methane are half of what conventional gasoline-powered cars produce, so even though it's just a stepping stone to true sustainability, it's a cleaner way of getting there.

Methods do exist for obtaining pure hydrogen gas that do not involve fossil fuels—electrolysis, for example, which uses electricity to split water into hydrogen and oxygen. But these methods are still cost-prohibitive; Los Alamos and other national labs are working to reduce the cost of renewably sourced hydrogen, which would help reduce the greenhouse-gas emissions of the entire energy sector.

Steam reforming, in addition to being fossil-fuel dependent, also presents a practical challenge to fuel-cell designers. The process isn't 100 percent efficient—a small proportion of other gaseous molecules remain in the hydrogen as impurities. These impurities, such as carbon monoxide and hydrogen sulfide, interfere with the precious platinum, covering its surface and thus poisoning it. This reduces the efficiency of the fuel cell and its lifespan too. As Los Alamos scientists work to develop new electrocatalysts, they are also working to understand how these materials will be affected by impurities in the hydrogen fuel. For example, for each type of impurity, how much can a fuel cell tolerate? Understanding that will help guide new hydrogen purification methods as well as the development of new catalyst materials.

Ultimately, all this fuel-cell technology has to be brought to market if it's to do any good. In order to help companies make maximum use of the fuel-cell research being done at Los Alamos, the DOE has set up a small business voucher program.



The chemistry inside a fuel cell is simple and compelling: Hydrogen is dissociated into electrons and hydrogen ions in the anode. The electrons provide electrical power and are then recombined with the hydrogen ions in the cathode, where oxygen is added, creating water as the only emission.

Automated vehicles, or self-driving cars, have tremendous potential for streamlining cities' transportation systems and boosting their occupants' quality of life. A city in which human-driven cars were replaced by automated vehicles may experience some impressive improvements: traffic jams and collisions could be largely avoided, fuel and time could be largely conserved, and people who can't drive now—blind people, young people, infirm people, intoxicated people—would be able to get where they need to go without endangering themselves and others. In order to quantify these hypothetical improvements, Los Alamos is bringing its error quantification and systems modeling expertise to the SMART Mobility consortium.

Small businesses can apply to get help from Los Alamos fuel-cell scientists to improve their fuel-cell technology and bring it into the marketplace. The Laboratory also wants to help big car companies understand how to improve their fuel cells. Each automotive company has its own program, with proprietary technology, so each company may use different pieces of what the Laboratory has to offer in different ways. By leveraging the expertise and technology present at Los Alamos and other national labs, car companies can rapidly move their fuel-cell products toward a cleaner transportation sector.

No driver necessary

Improving how cars are made and what they run on is, from an environmental standpoint, a giant step toward making the transportation system more sustainable. But what about the system itself? Truly sustainable transportation will require a switch to unmanned vehicles (popularly referred to as self-driving cars), which will be a complete paradigm shift involving changes in behavior for individuals, families, and cities. The newly formed System and Modeling for Accelerated Research in Transportation (SMART) Mobility consortium, a collaboration between the U.S. Departments of Energy and Transportation, supports national-lab research on transportation energy technologies and safety systems such as automated vehicles.

Unmanned vehicles are receiving a lot of attention these days—mostly for being hit by human-driven cars. But the reality of these vehicles is that they have the potential to streamline traffic, reduce energy consumption, improve safety, and boost quality of life. It's just hard to predict how much they will do these things before they have been deployed en masse. Los Alamos excels at uncertainty quantification and computer modeling and will, in collaboration with the NREL, bring unparalleled expertise to these efforts.

As a participant in the SMART Mobility consortium, Los Alamos will be modeling specific cities and regional settings to investigate how a shift to automated vehicles might impact human travel behavior, energy usage, city security, and greenhouse-gas emissions.

"The Lab's expertise in using computer simulations to identify important variables will help in orchestrating the shift to automated vehicles," says Joanne Wendelberger, Los Alamos scientist and liaison for the SMART Mobility consortium.

Sustainable transportation is indeed a multifaceted challenge. It will take metallurgists, chemists, geneticists, microbiologists, sociologists, computer simulators, time, money, and the will of society to make it happen. But it's inevitable. It has to be. Our current course, or rather our recently departed course, was always going to be a dead end.

—Eleanor Hutterer

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WHAT CAUSES CANCER?

WHY DO SOME NONSMOKERS GET LUNG CANCER while some heavy smokers live full lives cancer-free? Why do most cancers develop in adults while others affect children? Why are most skin moles benign—until they're not? In other words, what actually causes cancer?

The short answer is genetic mutations, which, in the case of cancer, generally cause one of two things to happen. Either they directly cause cells to proliferate too rapidly, or they inhibit the body's natural mechanisms to prevent overactive proliferation. But the long answer involves *which* mutations, how they come about, and how they can be repaired or treated. And despite decades of effort, the long answer has largely failed to emerge. Scientists have chipped away at a towering wall of opposition, carefully extracting clues with the genetic equivalent of a fossil brush and a rock hammer. Los Alamos's Ludmil Alexandrov, at long last, is carving it up with a light saber.

Ultraviolet light, tobacco, and other carcinogens are known to trigger DNA mutations that cause cancer. But which mutations and why?

Alexandrov uses advanced supercomputers at Los Alamos to examine the full genomes of tumor cells (alongside noncancerous blood cells from the same individuals for reference) and identify mutational patterns. To date, he has analyzed the genomes from 12,023 samples spanning 40 different human cancers and identified more than 8 million distinct mutations. But mutations alone do not a cancer make, and from these 8 million mutations, he has identified 30 "mutational signatures"—recurring combinations of mutations that act like genetic fingerprints for various human cancers. Some signatures correspond to known cancer-causing defects in the genome. Others correspond to known or suspected carcinogens. Others still remain a complete mystery.

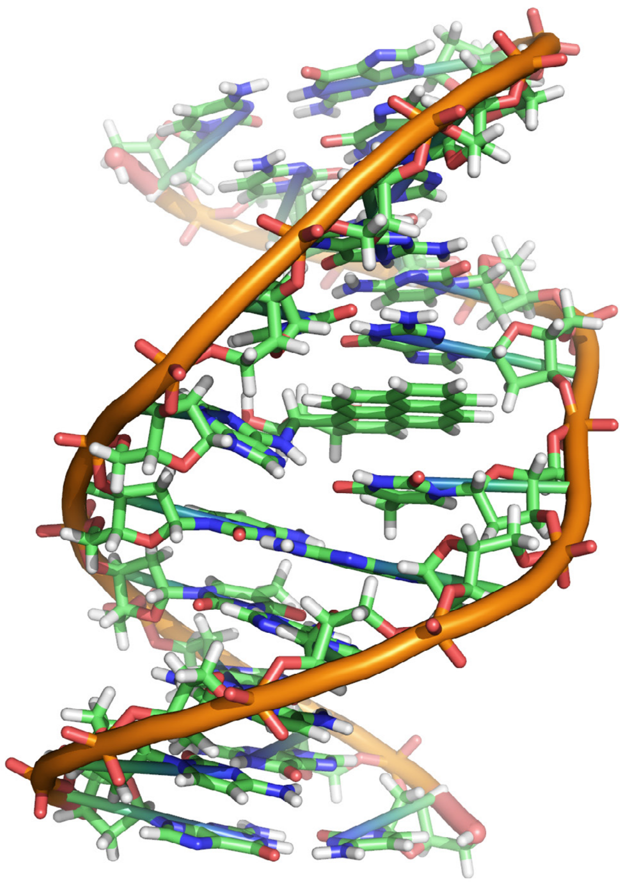
Cancer's humble origins

"Most people think of cancer as something gone wrong," says Alexandrov, "and that's definitely true. But in a sense, it's also something gone *too* right." He explains that all the cells that comprise our multicellular bodies have an evolutionary history from single-celled organisms. Those organisms thrived when they were able to outcompete neighboring cells. But within a multicellular organism, that's not so advantageous. "You don't want an individual cell in the bladder or pancreas outcompeting all its neighbors."

Normally, the body's immune system prevents individual cells from getting out of control, but such immunity is imperfect. For one thing, immune cells didn't evolve to fight modern-world cellular insults, such as tobacco, asbestos, or x-rays. For another, the immune system can become compromised by illness or immunosuppressant medications. Yet even in individuals with healthy immune systems facing naturally occurring carcinogens, immune cells, like other cells, become less effective with age. And while this, too, can be seen as a something gone right—such as when immune and other cells die or go dormant to prevent their accumulated damage from affecting the rest of the body—it still means that, with age, the immune system weakens as mutations proliferate. At some point, the problematic mutations outpace the immune system.

Most mutations, however, are not problematic. During human cellular replication, there are typically more than 50,000 naturally occurring errors, and nearly all are automatically corrected during the process. Those that remain are bona fide mutations, yet they rarely cause any trouble. Even mutations caused by external exposures, such as chemical carcinogens or ultraviolet (UV) light, without an intense or sustained degree of exposure, rarely cause trouble. Part of the reason is that only about 1.5 percent of human DNA actually encodes for useful proteins. And even when a mutation hits that 1.5 percent, it still amounts to a very small discrepancy. It might mess up just one DNA base pair (one rung in the DNA "ladder") out of the hundreds, thousands, or tens of thousands that make up a single gene. Such a small glitch may not actually prevent the gene, or the protein it encodes, from functioning properly. And even if the mutation were to cripple the gene, it's only one of about 30,000 human genes. Chances are, the cell can get by without it.

The problem arises when many of these mutations combine together. A cell copies its DNA when it divides, including its acquired mutations, so all of its daughter cells have those same mutations. Thirty generations of harmless mutations down the line, say, a new mutation impairs another gene. After a couple thousand generations, the descendent cells now have a number of flaws in each of several genes. This becomes a problem if the complex pattern of accumulated



Genetic mutations can arise as a result of natural copying errors during DNA replication or as the result of an external disruption, such as exposure to radiation or a carcinogenic chemical. Here, one "rung" of the DNA "ladder" has been broken by a modified form of benzo[a]pyrene (planar green and white molecule at center), found in cigarette smoke. The carcinogenic molecule binds to the base guanine (the G in genetic code). During replication, the guanine is no longer recognized and is erroneously interpreted as thymine (T).
CREDIT: Zephyris/Wikimedia Commons

mutations includes two complementary functional effects: causing excessive replication and inhibiting the genes that suppress excessive replication.

Yet such a confluence of harmful mutations still does not constitute "real" cancer. In general, when one cell undergoes excessive replication, the body's immune system takes notice and deploys some manner of antidote. This might describe a benign skin mole, for example; a damaged cell proliferates until the body finds a way to halt its growth. To pose a danger, the mole must then acquire mutations that allow it to break through the internal cellular reguation as well as the immune system's defenses and resume replicating uncontrollably. At this point, it's skin cancer.

In general, a localized cancer of this sort can become life threatening in two ways. Either it grows to the point of effectively incapacitating the organ it formed within (as in liver cancer) or another mutation causes it to move beyond its organ of origin and invade other parts of the body. In the case of a mole-turned-malignant, this means moving beyond the skin and replicating uncontrollably in other organs, which are only equipped to fight their own internal cancers, not cancers of the skin. Such a metastatic cancer may start to appear all over the body, at which point the cellular proliferation proceeds unimpeded, and the patient is unlikely to survive. In fact, metastases cause 90 percent of human cancer deaths.

Tumor fingerprinting

While random mutations from ordinary DNA replication during one's lifetime can cause cancer, the risk is much greater with exposure to cancer-causing agents. UV light and nuclear radiation, for example, can induce mutations in DNA by breaking its internal bonds in such a way that they reconnect incorrectly. Chemical carcinogens similarly disfigure DNA.

Cigarette smoking, for example, reliably produces the chemical carcinogen benzo[a]pyrene. A natural product of incomplete combustion—also found in coal tar, fireplace chimneys, and grilled foods—benzo[a]pyrene undergoes chemical changes in the body and subsequently bonds to the base guanine, the "G" in DNA's "ACGT" genetic code. This distorts the double helix. When the enzymes that carry out DNA replication encounter the distortion and don't know what to make of it, they effectively take a guess. But they guess wrong, assuming it should be a T, which pairs with A, instead of a G, which pairs with C. That's the mutation.

Different carcinogens act differently, but the resulting DNA mutation, following replication, often takes the form of a base-pair substitution like this. Alexandrov identifies each such mutation by its incorrect genetic character substitution, as in G→T, together with the characters that come before and after for context, as in CGG→CTG. Characterized in this fashion, he identifies 96 possible mutation classes and then goes hunting for them in genomes pulled from cancerous human cells. He obtains thousands upon thousands of these genomes from the International Cancer Genome Consortium, which maintains a large and growing database of cancer genomics data, and processes them through a data-analysis pipeline he developed, running on the Laboratory's Institutional Computing supercomputers.

"There are few places in the world that can handle the petabytes of data," says Alexandrov. "For any given run of the analysis, a normal computer would have to chew on it for months at least. Here at Los Alamos, I can do it in a day."

The supercomputer analysis confirmed what Alexandrov already knew, that it's not just a single genetic character substitution that characterizes a cancer. Rather, it's a complex blend of the 96 possible mutation classes, each with different occurrence rates. In the language of linear algebra, he creates a 96-term linear combination of mutation classes—how much class 1? how much 2? how much 96?—for each recurring pattern of mutations in his cancer genome pool. Each constitutes a mutational signature: a complicated indication of one or more types of cancer (or susceptibility to it). In turn, the cancer genomes studied—each unique to a particular cancer patient—are themselves linear combinations of mutational signatures.

Alexandrov has identified and published 30 distinct mutational signatures to date and correlated them across the 40 different types of cancer represented in the genome pool.

Signatures 1 and 5, for example, show up across the board; all 40 types of cancer show these mutational signatures. Signature 7 is consistent with classic UV-induced mutations and shows up in skin melanomas as well as oral, head, and neck cancers. Signatures 23 and 24, both of unknown origin, show up in liver cancer only.

You don’t want an individual cell in the bladder or pancreas outcompeting all its neighbors.

How does someone acquire these mutational signatures? In some cases, it’s relatively easy to figure out, as with certain G→T substitutions in cigarette smokers’ DNA. Indeed, Alexandrov was able to identify different signatures particular to smokers and nonsmokers in lung cancers, as well as signatures that distinguish between smoking tobacco and chewing it. Other signatures—numbers 6, 15, 20, and 26—can be positively associated with defective DNA-mismatch repair mechanisms. And Signature 1 is apparently age-related, operating by a particular mechanism associated with cell mitosis. In other cases, there are no answers yet. Signature 5 is also likely to be age related but isn’t associated with any known mechanism. And of 13 signatures found to correlate with breast cancer, six are similarly unknown. In total, 11 of the 30 signatures have no known—or even suspected—cause.

Rather than being discouraged by so many mutational signatures of unknown cause, Alexandrov seems to value them. “You have to see the unknowns as good news,” he says. “We’re discovering completely new things about the genetic basis for cancer. This is progress. Identifying the causes and therapies will follow.”

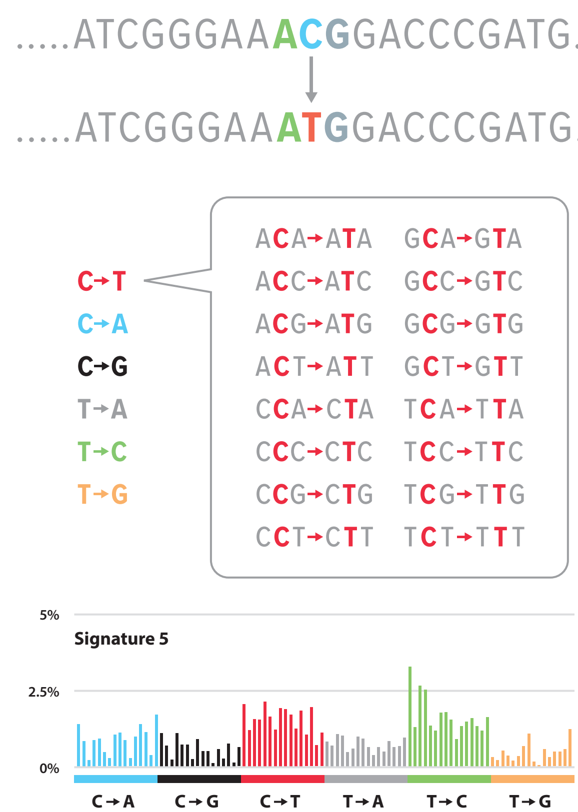
From theory to therapy

Some cancer-causing mutations can be inherited, rather than acquired. For instance, mutations in two well-studied tumor-suppressor genes, *BRCA1* and *BRCA2*, have long been known to associate with breast and ovarian cancers, leading some women to have their breasts or ovaries surgically removed rather than risk those tumors showing up someday. These hereditary mutations cause Signature 3. Together, the inherited and acquired mutations associated with Signature 3 constitute the combination of genetic risk, environmental exposure, and just plain bad luck that brings about actual breast and ovarian cancers.

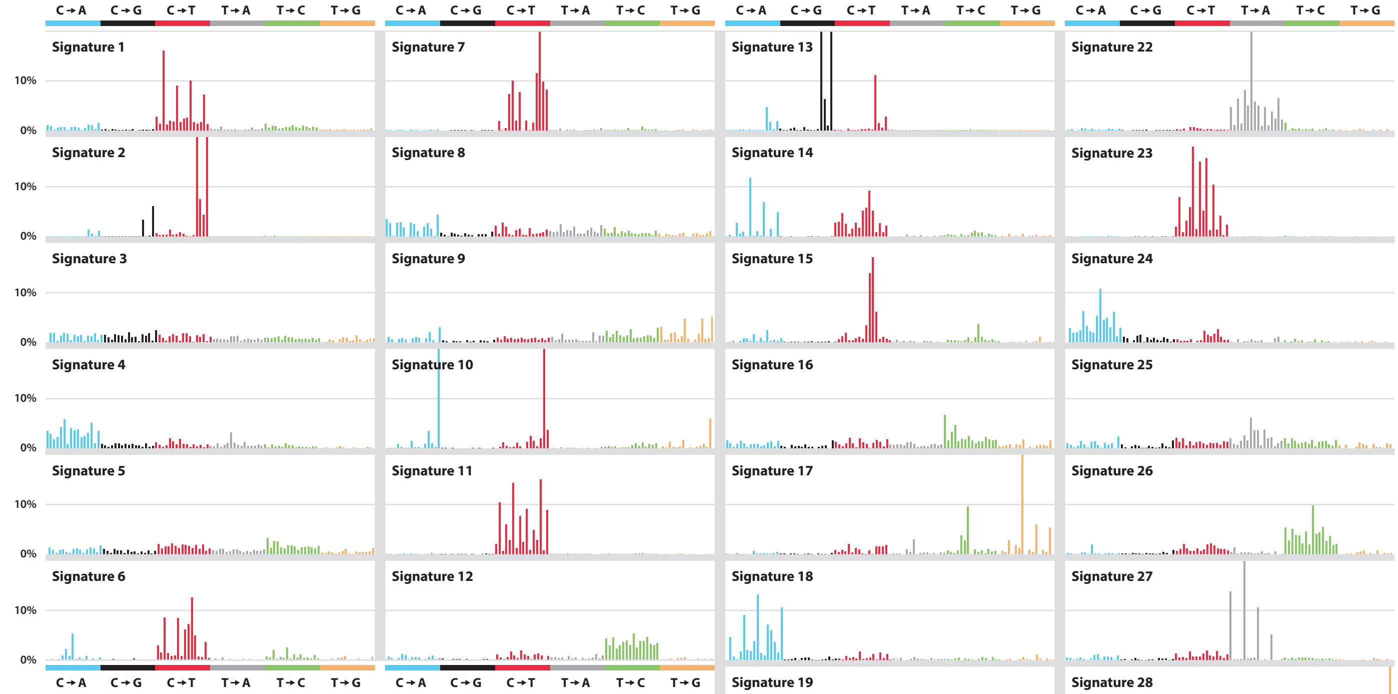
Importantly, Alexandrov’s analysis recently revealed that Signature 3 also correlates significantly with pancreatic and gastric (stomach) cancers.

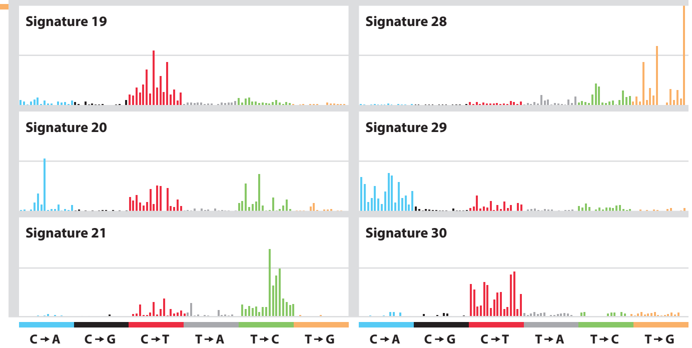
“Gastric cancer is the third-leading cause of cancer-related deaths worldwide,” Alexandrov says. “This discovery suggests a direct way to treat at least some of them.” Previous research classified patients with pancreatic cancers exhibiting a Signature 3 genetic profile (about 8 percent of them) as exceptional responders to platinum-based chemotherapy drugs. The same now seems likely to prove true for 10 percent of stomach cancers. It may also help tailor more effective treatments for about a third of breast and ovarian cancer patients—the ones matching Signature 3. The discovery also suggests that another class of drugs for treating ovarian cancer, PARP inhibitors, are likely to help with these gastric and pancreatic cancers.

Of course, treating cancer is a tricky and oftentimes discouraging business, and developing drugs that target a genetic abnormality is no exception. Several things have to go right if the drug is to make any significant difference. First, the particular genetic defect it addresses has to be utterly critical to the growth of the cancer, not just part of the mutational signature that’s along for the ride. Second, it has to be possible to create a drug that counteracts the



A section of the human genome develops a mutation by incorrectly replacing one base with another, such as cytosine becoming thymine (C→T, top). Taking into account the bases immediately preceding and following the swapped base for context, each of six possible swaps generates 16 possible variations of that mutation class (center), making 96 possible variations in all. (Because of the way bases pair in DNA—C with G and T with A—the six swaps shown intrinsically include their inverses; e.g., C→T includes G→A.) A mutational signature, identified by its repeated occurrence in tumor genomes from many cancer patients, is constructed from a tally of how many of its component mutations correspond to each of the 96 mutational variants. Displayed as a column graph (bottom), 96 columns wide, is a mutational signature observed in all 40 different types of human cancer included in the study.





In more than 12,000 cancer genomes covering 40 human cancers, Los Alamos supercomputer analyses revealed 30 distinct mutational signatures. Some are present in all 40 cancers; others are present in just a few. Nineteen of the 30 have at least one known or suspected cause (such as Signature 7, caused by ultraviolet light); the other 11 have yet to be identified. In principle, any cancer relying on a certain mutational signature to make it over-proliferate may be vulnerable to a drug designed to counteract the effects of that signature.

defect in some fashion, which isn't always the case. Third, even with an effective drug, who's to say the temporarily thwarted cancer won't find another defect to exploit, so it can resume its uncontrolled proliferation? This could happen either because the cancer follows a natural progression from one problem to another or because the treatment itself encourages drug resistance in the tumor cells it fails to kill.

Those caveats notwithstanding, treatments based on tumor genetics have had a real impact, reliably, if modestly, extending the lives of cancer patients. And the Signature 3 discovery is particularly promising because it implies a treatment strategy using drugs that already exist.

Yet it's not just drug identification and development that the research may benefit. Alexandrov has shown that Signatures 1 and 5 constitute "mutational molecular clocks"—timekeepers for processes that mutate DNA on a regular schedule as a person ages. Knowledge of them may allow doctors to accurately assess the time-progression of numerous cancers, which is likely to help in selecting the optimal therapy among imperfect choices.

"The point is, we're obtaining lots of new information about the exact mutations that cause different cancers," says Alexandrov. "Molecular clocks and treatments for gastric and pancreatic cancers are just the beginning. We don't yet know all the avenues for discovery and treatment that genetic fingerprinting will open up."

Of course, to anyone suffering from cancer or from the loss of a cancer victim, such opportunities for discovery could seem like only a distant hope at best. And no wonder—at seemingly every turn, cancer has shown itself to be a hardier foe than anticipated. Yet after so many frustrating decades of trying to figure out what makes cancer tick—and more importantly, what can make it stop ticking—investigators might now be getting what they've needed most: a solid lead. LDRD

—*Craig Tyler*

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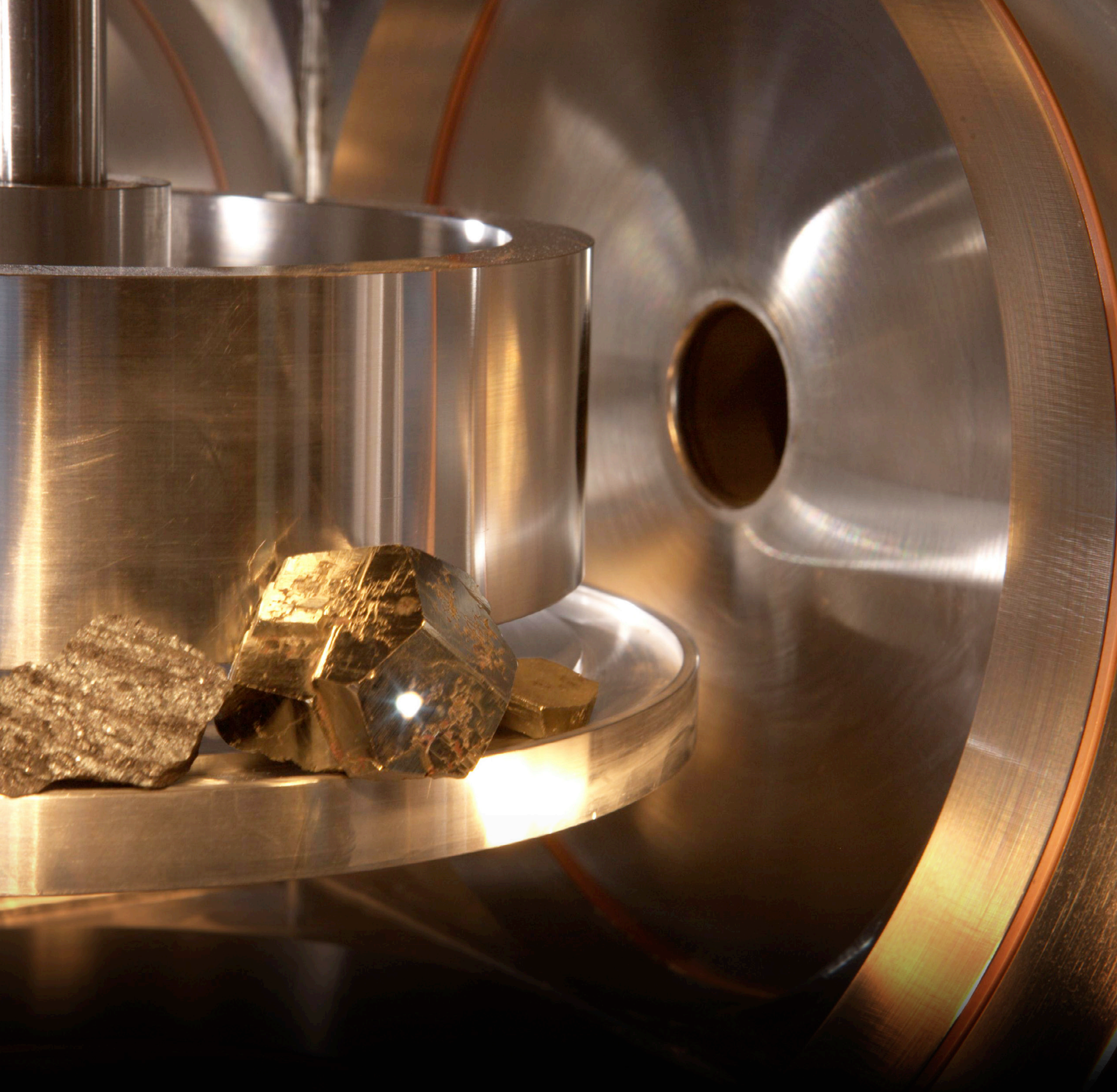

Laser-induced Breakdown Spectroscopy (LIBS) is an elemental analysis tool that was developed largely at Los Alamos National Laboratory. A small but powerful laser is used to ablate a tiny portion of a sample's surface, creating a plume of excited atoms and molecules that emit light at characteristic wavelengths. A spectrometer built into the tool resolves the wavelengths and measures the intensity of the emissions to determine the identity and concentration of elements in the sample. Here, a LIBS instrument is seen probing (bright spot) a piece of iron pyrite at Los Alamos shortly before the instrument was installed on the Mars rover *Curiosity*. For more about LIBS at Los Alamos, see "Little Laser, Big Science" on page 14.

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Farolitos or luminarias? For centuries, New Mexico residents have passionately disagreed on the correct name for these little lanterns, each made from a paper bag containing sand and a lit candle. During the holiday season, they are a spectacle to be seen, with thousands lining walkways and adorning the tops of buildings and walls. This tradition is rooted in the state's Spanish heritage and culminates on Christmas Eve, when crowds of residents and tourists bundle up for a nighttime stroll to see friends, family, and all the flickering lights.

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